of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:53:55 ON 31 JAN 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	1.05	1.05

FILE 'REGISTRY' ENTERED AT 10:57:03 ON 31 JAN 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 JAN 2007 HIGHEST RN 918865-48-2
DICTIONARY FILE UPDATES: 30 JAN 2007 HIGHEST RN 918865-48-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

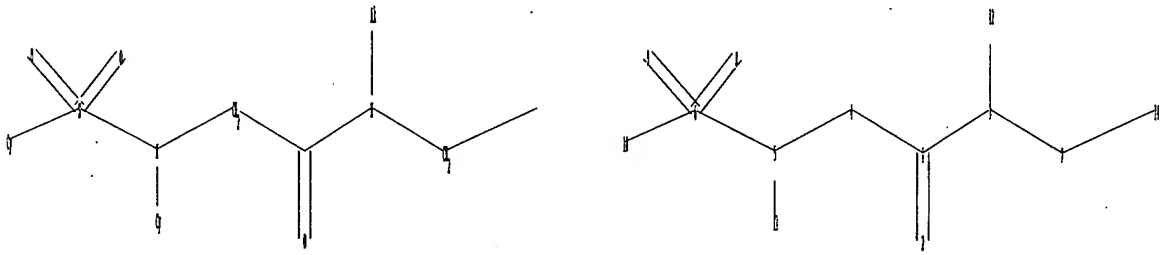
TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10529637-exam-broad.str



chain nodes :
1 2 3 4 5 6 7 8 9 10 11 12 14
chain bonds :
1-2 1-3 1-4 3-7 3-12 4-5 5-6 5-11 6-8 6-9 6-10 7-14
exact/norm bonds :
1-2 1-3 1-4 3-7 3-12 4-5 5-6 5-11 6-8 6-9 6-10 7-14

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:Atom 11:Atom 12:CLASS 14:CLASS
Generic attributes :
12:
Saturation : Saturated

STN STRUCTURE SEARCH.

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptayvv1621

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 4	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 5	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS 6	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS 7	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 8	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 9	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS 10	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS 11	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS 12	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS 13	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 14	DEC 18	CA/CAplus patent kind codes updated
NEWS 15	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 16	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS 17	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS 18	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 19	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 20	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 21	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 22	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 23	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 24	JAN 29	PHAR reloaded with new search and display fields
NEWS 25	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that specific topic.

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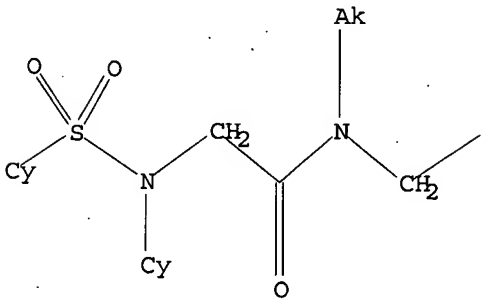
Number of Carbon Atoms : less than 7

Element Count :
Node 12: Limited
C,C1-6

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 10:57:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2068 TO ITERATE

96.7% PROCESSED 2000 ITERATIONS 28 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 38633 TO 44087
PROJECTED ANSWERS: 257 TO 901

L2 28 SEA SSS SAM L1

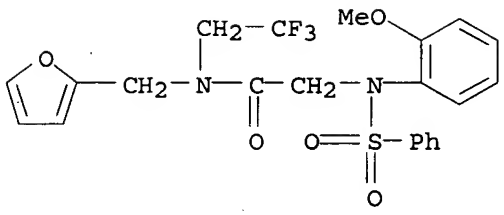
=> s l1 full
FULL SEARCH INITIATED 10:57:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 40272 TO ITERATE

100.0% PROCESSED 40272 ITERATIONS 507 ANSWERS
SEARCH TIME: 00.00.01

L3 507 SEA SSS FUL L1

=> d l3 scan

L3 507 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C22 H21 F3 N2 O5 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.55	173.60

FILE 'CAPLUS' ENTERED AT 10:58:27 ON 31 JAN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 31 Jan 2007 VOL 146 ISS 6
FILE LAST UPDATED: 30 Jan 2007 (20070130/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
L4 16 L3

=> s l4 not py > 2004
2662812 PY > 2004
L5 11 L4 NOT PY > 2004

=> s l5 not 529637
0 529637
L6 11 L5 NOT 529637

=> d l6 abs ibib hitstr 1-
YOU HAVE REQUESTED DATA FROM 11 ANSWERS - CONTINUE? Y/(N):y

L6 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
AB The authors report the synthesis of 7α-substituted β-estradiol derivs. bearing side chains terminated with cholesterol and 3β-cholesterylamine. These chimeric compds. were designed to exhibit

high affinity for estrogen receptors (ERs) and cellular plasma membranes to potentially enable regulated uptake of ERs by mammalian cells. Evaluation with recombinant yeast reporting compound-mediated ER dimerization revealed potencies similar to the antiestrogen ICI 182780. Compds. that efficiently deliver dominant neg. ERs into cells may provide novel therapeutics against breast cancers.

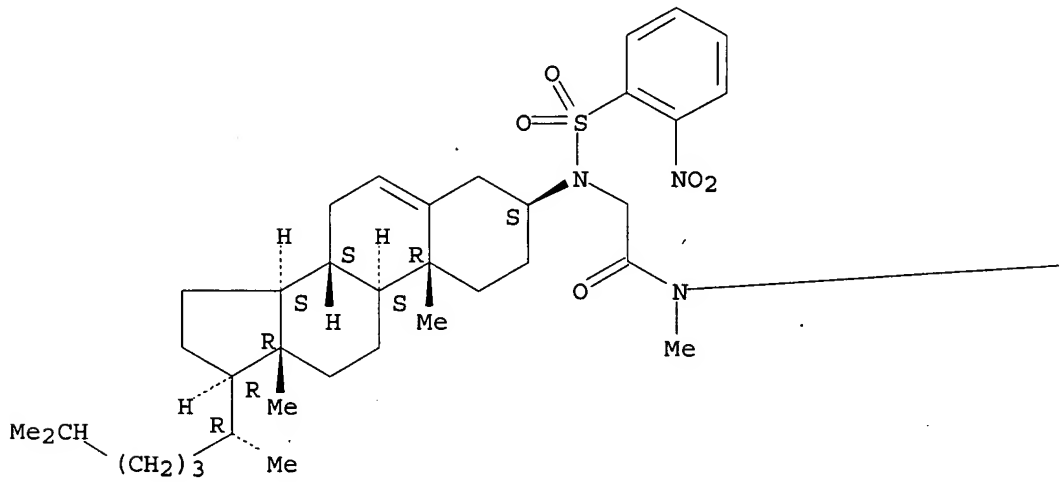
ACCESSION NUMBER: 2002:14237 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 136:216932
TITLE: Synthesis of Chimeric 7α-Substituted Estradiol Derivatives Linked to Cholesterol and Cholesterylamine
AUTHOR(S): Hussey, Stephen L.; He, Enfei; Peterson, Blake R.
CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Organic Letters (2002), 4(3), 415-418
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:216932

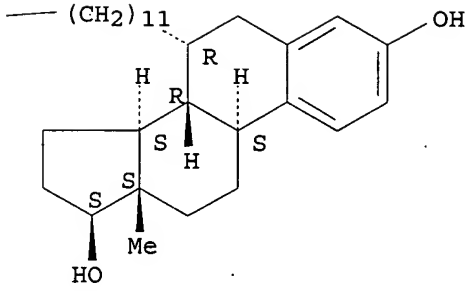
IT 402570-31-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and estrogen receptor affinity of estradiol-cholesterol and -cholesterylamine derivs. as potential anticancer agents)

RN 402570-31-4 CAPLUS
CN Acetamide, 2-[(3β)-cholest-5-en-3-yl[(2-nitrophenyl)sulfonyl]amino]-N-[11-[(7α,17β)-3,17-dihydroxyestra-1,3,5(10)-trien-7-yl]undecyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

AB X1X2X3CC(R1)(ArYR2)CX4X5X6 (Ar = aryl; R1 = OH, CO2H, alkoxy, alkylcarbonyloxy, heteroalkyloxy, etc.; R2 = alkyl, heteroalkyl, aryl, aralkyl; X1-X6 = H, alkyl, heteroalkyl, F, Cl; Y = NR12SOm, NR12CO, NR12CONR13, NR12CO2, etc.; m = 1, 2; R12, R13 = H, alkyl, heteroalkyl, aryl, aralkyl, etc.; with provisos), were prepared Thus, 4-(hexafluoro-2-hydroxyisopropyl)aniline in MeOH was treated with PhSO2Cl to give 4-[HO(CF3)2C]C6H4NHSO2Ph. The latter showed LXRα with EC50 <2 μM.

ACCESSION NUMBER: 2000:666587 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 133:237693
TITLE: Preparation of bis(trifluoromethyl)hydroxymethylbenzenesulfonamides, -ureas, and -carbamates as liver X receptor modulators.
INVENTOR(S): Li, Leping; Medina, Julio C.; Hasegawa, Hirohiko; Cutler, Serena T.; Liu, Jiwen; Zhu, Liusheng; Shan, Bei; Lustig, Kevin
PATENT ASSIGNEE(S): Tularik Inc., USA
SOURCE: PCT Int. Appl., 113 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000054759	A2	20000921	WO 2000-US6611	20000315
WO 2000054759	A3	20010215		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,

CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6316503	B1	20011113	US 2000-525861		20000314
CA 2367595	A1	20000921	CA 2000-2367595		20000315
EP 1161233	A2	20011212	EP 2000-914958		20000315
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
JP 2002539155	T	20021119	JP 2000-604835		20000315
PRIORITY APPLN. INFO.:			US 1999-124525P	P	19990315
			WO 2000-US6611	W	20000315

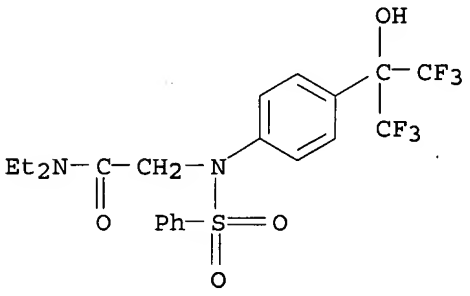
OTHER SOURCE(S): MARPAT 133:237693

IT 293754-48-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bis(trifluoromethyl)hydroxymethylbenzenesulfonamides, -ureas, and -carbamates as liver X receptor modulators)

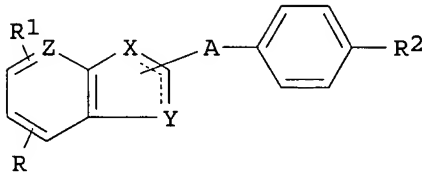
RN 293754-48-0 CAPLUS

CN Acetamide, N,N-diethyl-2-[(phenylsulfonyl)[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]amino]- (9CI) (CA INDEX NAME)



L6 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

GI



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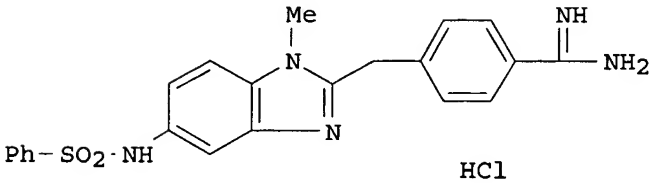


HCl II

AB Title compds. [I; R = 5-C6H5SO2NH, 6-C6H5SO2NH, 5-C6H5NHSO2, 5-C6H5SO2N(CH2COOEt), 5-C6H5SO2N(CH3), 5-C6H5N(CH2CH2CH2COOEt)CO, 5-C6H5,

CH3N(C6H5)CO, 8; R1 = H, 7-CH3, 3-Br, 3-EtO; R2 = C(:NH)NH2; A = CH2, NH; X = CH, MeN, EtOCOCH2CH2N, O, S, NCH2CO2H; Y = N, CH, CH:CH; Z = CH, N; dotted bond = single, double in relation to X; A is attached at 2,or 8 position depending on the heterocyclic ring] and their tautomers, stereoisomers, mixts. and their physiol. compatible salts with inorg. or organic acids or bases are prepared and title compds in which R2 is a cyano group, present valuable intermediate products for the production of the remaining compds. of the general formula I, with R2 is amidino, which have valuable pharmacol. properties, especially an antithrombotic activity. Thus, the title compound II was prepared

ACCESSION NUMBER: 1999:511140 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 131:157771
TITLE: Preparation of five-membered, benzo-condensed heterocycles as antithrombotics
INVENTOR(S): Ries, Uwe; Hauel, Norbert; Mihm, Gerhard; Priepke, Henning; Binder, Klaus; Stassen, Jean Marie; Wienen, Wolfgang; Zimmermann, Rainer
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma Kg, Germany
SOURCE: PCT Int. Appl., 250 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

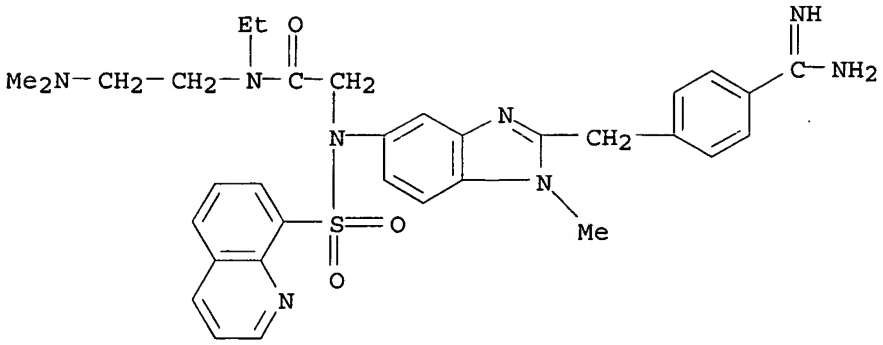
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9940072	A1	19990812	WO 1999-EP537	19990128
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19804085	A1	19990805	DE 1998-19804085	19980203
DE 19834325	A1	20000217	DE 1998-19834325	19980730
CA 2319494	A1	19990812	CA 1999-2319494	19990128
AU 9927201	A	19990823	AU 1999-27201	19990128
EP 1060166	A1	20001220	EP 1999-907437	19990128
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002502844	T	20020129	JP 2000-530502	19990128

PRIORITY APPLN. INFO.:
DE 1998-19804085 A 19980203
DE 1998-19834325 A 19980730
WO 1999-EP537 W 19990128

OTHER SOURCE(S): MARPAT 131:157771

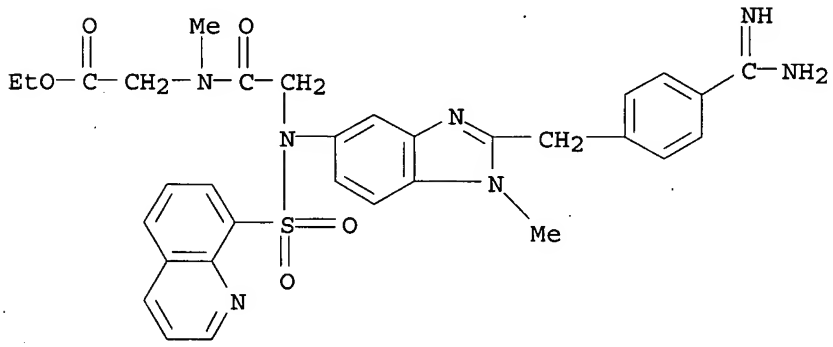
IT 236415-28-4P 236415-95-5P 236415-97-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of five-membered benzo-condensed heterocycles as antithrombotics)

RN 236415-28-4 CAPLUS
CN Acetamide, 2-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl](8-quinolinylsulfonyl)amino]-N-[2-(dimethylamino)ethyl]-N-ethyl-, dihydrochloride (9CI) (CA INDEX NAME)



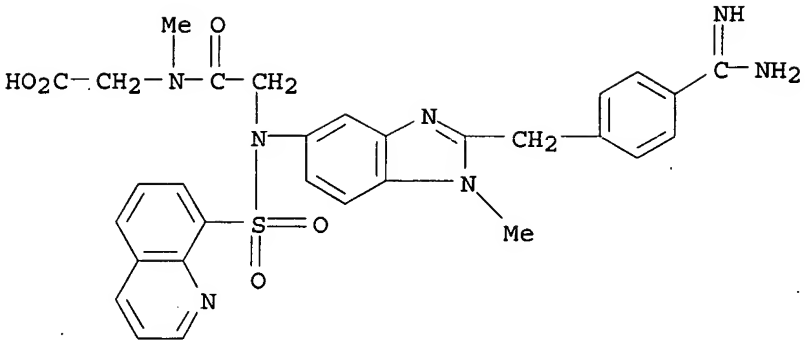
● 2 HCl

RN 236415-95-5 CAPLUS
CN Glycine, N-[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 236415-97-7 CAPLUS
CN Glycine, N-[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

AB Approx. 300 antithrombotic title compds. such as 4-[5-[N-(8-quinolylsulfonyl)-N-(carboxymethyl)amino]-1-methyl-1H-benzimidazol-2-ylmethyl]benzamidine hydrochloride (I), 4-[5-[N-(benzenesulfonyl)-N-[2-(dimethylamino)ethyl]amino]-1-benzyl-1H-benzimidazol-2-ylmethyl]benzamidine dihydrochloride, 4-[5-[N-(3-carboxypropionyl)-N-(cyclopentyl)amino]-1-methyl-1H-benzimidazol-2-ylmethyl]benzamidine hydrochloride (II), and 4-[5-[N-(8-quinolylsulfonyl)-N-(carboxymethyl)amino]-1-methyl-1H-benzothiazol-2-ylmethyl]benzamidine hydrochloride were prepared by standard methods. The ED200 in μM for I was 0.92 and for II was 0.82. Formulations for the antithrombotics were given.

ACCESSION NUMBER: 1999:505930 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 131:157761
TITLE: 5-Membered heterocyclic condensed benzo derivatives, their preparation, and their use as drugs
INVENTOR(S): Ries, Uwe; Hauel, Norbert; Mihm, Gerhard; Priepke, Henning; Binder, Klaus; Stassen, Jean Marie; Wienen, Wolfgang; Zimmermann, Rainer
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany
SOURCE: Ger. Offen., 94 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19804085	A1	19990805	DE 1998-19804085	19980203
CA 2319494	A1	19990812	CA 1999-2319494	19990128
WO 9940072	A1	19990812	WO 1999-EP537	19990128
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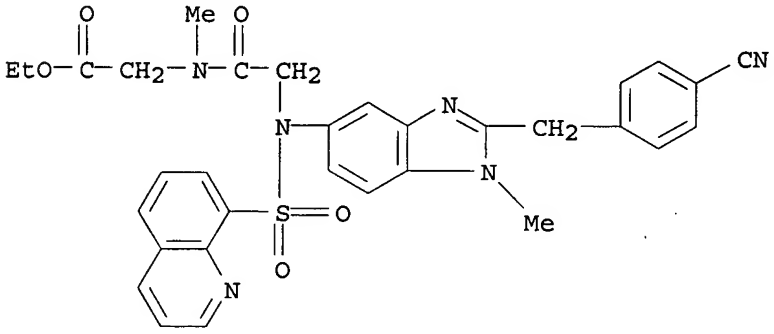
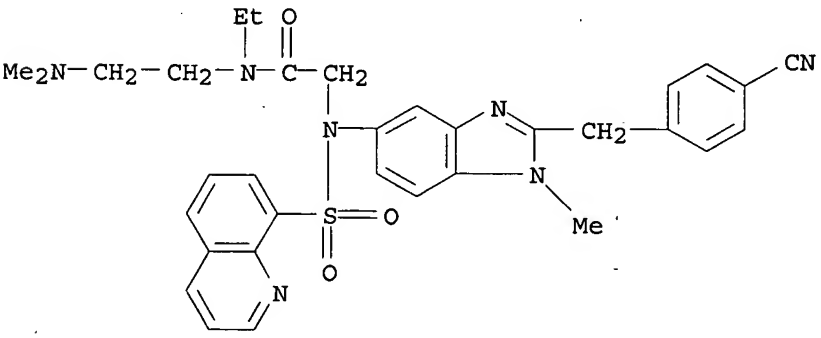
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9927201	A	19990823	AU 1999-27201	19990128

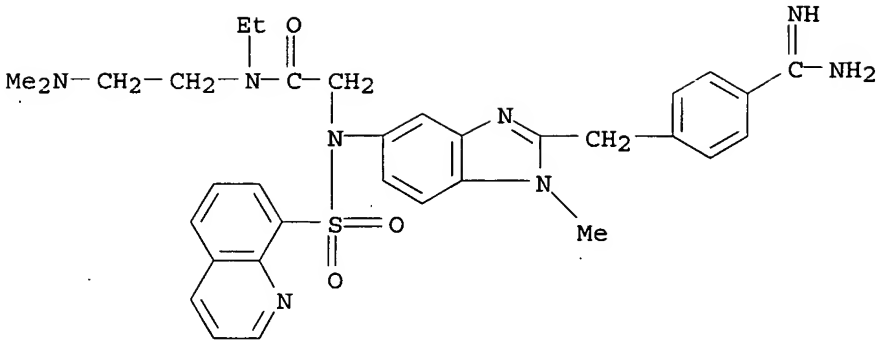
EP 1060166 A1 20001220 EP 1999-907437 19990128
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO
JP 2002502844 T 20020129 JP 2000-530502 19990128
US 6114532 A 20000905 US 1999-243200 19990202
PRIORITY APPLN. INFO.: DE 1998-19804085 A 19980203
US 1998-77694P P 19980312
DE 1998-19834325 A 19980730
WO 1999-EP537 W 19990128
OTHER SOURCE(S): MARPAT 131:157761
IT 237751-41-6 237752-24-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and antithrombotic activity of benzimidazolylmethylbenzamidines)
RN 237751-41-6 CAPLUS
CN Glycine, N-[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 237752-24-8 CAPLUS
CN Acetamide, 2-[[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-5-yl](8-quinolinylsulfonyl)amino]-N-[2-(dimethylamino)ethyl]-N-ethyl- (9CI) (CA INDEX NAME)

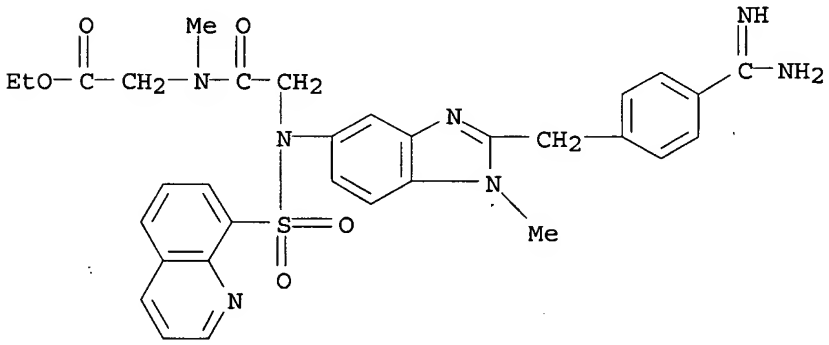


IT 236415-28-4P 236415-95-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and antithrombotic activity of benzimidazolylmethylbenzamidines)
RN 236415-28-4 CAPLUS
CN Acetamide, 2-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl](8-quinolinylsulfonyl)amino]-N-[2-(dimethylamino)ethyl]-N-ethyl-, dihydrochloride (9CI) (CA INDEX NAME)



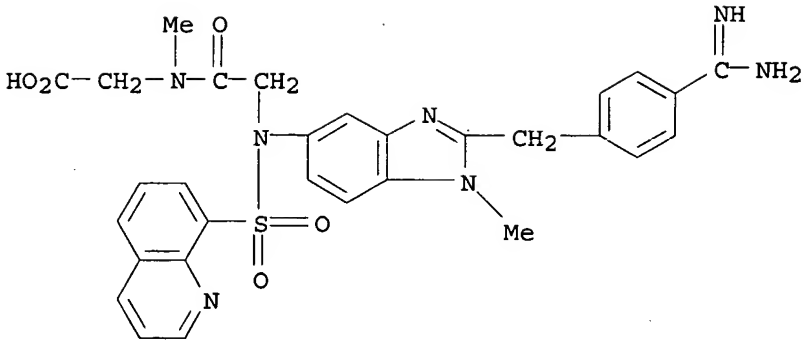
●2 HCl

RN 236415-95-5 CAPLUS
CN Glycine, N-[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



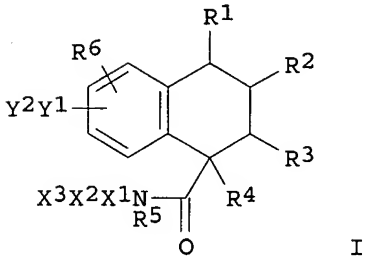
● HCl

IT 236415-97-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antithrombotic activity of benzimidazolylmethylbenzamidines)
RN 236415-97-7 CAPLUS
CN Glycine, N-[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L6 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
GI



I

AB Title compds. [I; R1-R4 = H, or R1, R2 = H, R3R4 = double bond, or R1R2 and R3R4 = double bonds; R5 = H, alkyl; R6 = H, F, Cl, Br, alkyl; X1 = alkylene; X2 = phenylene, cycloalkylene, thienylene, oxazolylene, thiazolylene, imidazolylene, pyridinylene, pyrimidinylene, pyrazinylene, pyridazinylene; X3 = cyano, amino, 2-amino-1H-imidazol-4-yl, etc.; Y1 = O, RbN, RbNSO2, RbNCO, etc.; Rb = H, (substituted) alkyl, phenylalkyl, naphthylalkyl, aminocarbonyl, etc.; Y2 = alkyl, cycloalkyl, (substituted) aminocarbonylalkyl, Ph, naphthyl, pyrrolyl, thiazolyl, thienyl, pyridinyl, etc.], were prepared Thus, Et [2-[quinolin-8-sulfonyl-[5-(carbamidoylbenzylcarbamoyl)-3,4-dihydronaphthalen-2-yl]amino]acetylamino]acetate hydrochloride showed a thrombin time ED200 = 0.009 μM.

ACCESSION NUMBER: 1999:384101 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 131:44664
TITLE: Preparation of carbamoylnaphthalenes as thrombin inhibitors.
INVENTOR(S): Soyka, Rainer; Heckel, Armin; Lehmann-Lintz, Thorsten; Walter, Rainer; Wienen, Wolfgang; Stassen, Jean Marie
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany
SOURCE: Ger. Offen., 92 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19754490	A1	19990610	DE 1997-19754490	19971209
WO 9929670	A2	19990617	WO 1998-EP7958	19981208
WO 9929670	A3	19990910		

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT; BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

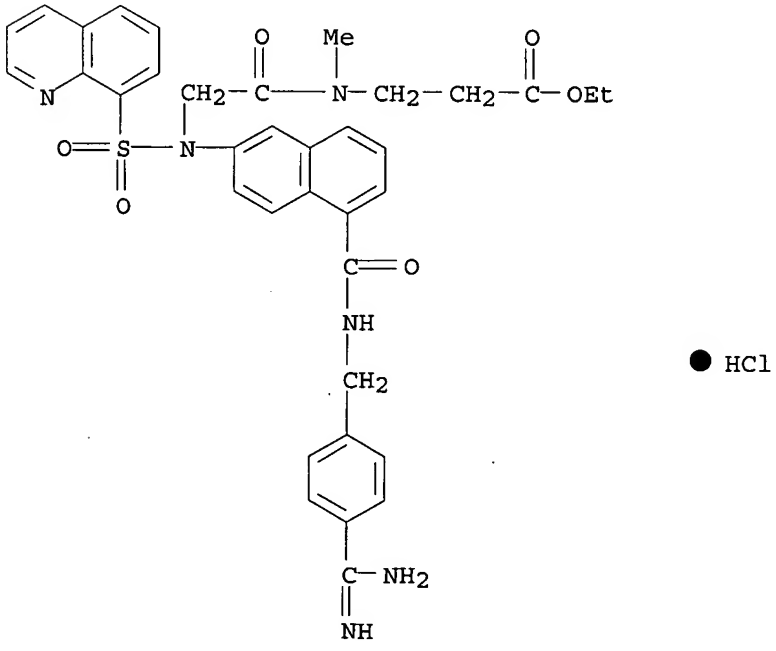
AU 9918773	A	19990628	AU 1999-18773		19981208
PRIORITY APPLN. INFO.:			DE 1997-19754490	A	19971209
			WO 1998-EP7958	W	19981208

OTHER SOURCE(S): MARPAT 131:44664

IT 227276-66-6P 227276-68-8P 227276-69-9P
227276-71-3P 227276-76-8P 227276-78-0P
227276-79-1P 227276-81-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of carbamoylnaphthalenes as thrombin inhibitors)

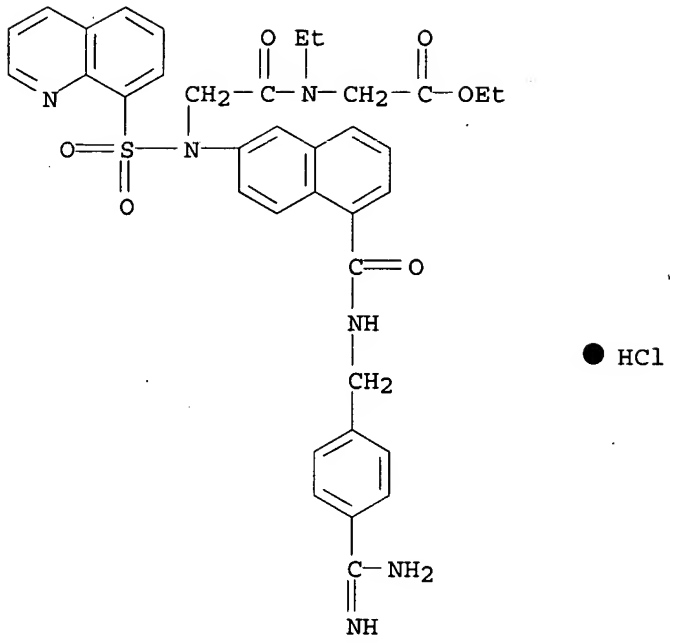
RN 227276-66-6 CAPLUS

CN β-Alanine, N-[5-[[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

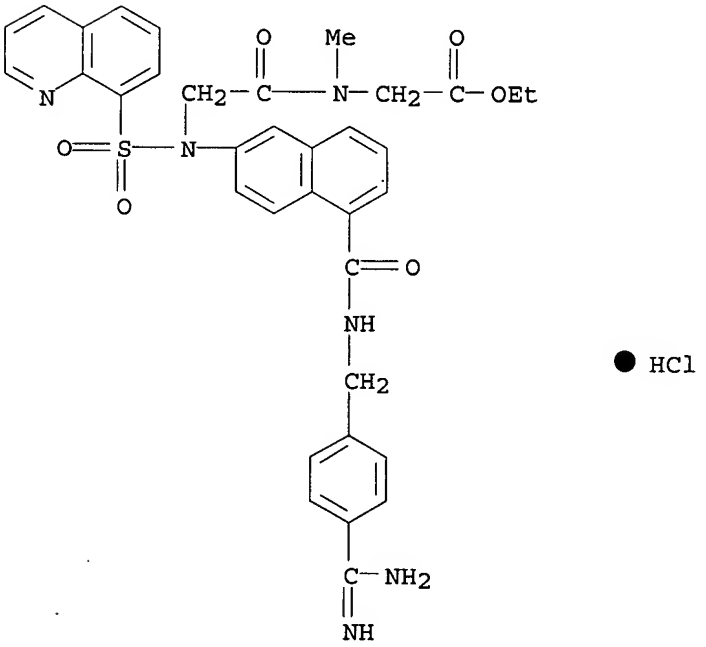


RN 227276-68-8 CAPLUS

CN Glycine, N-[5-[[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-ethyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

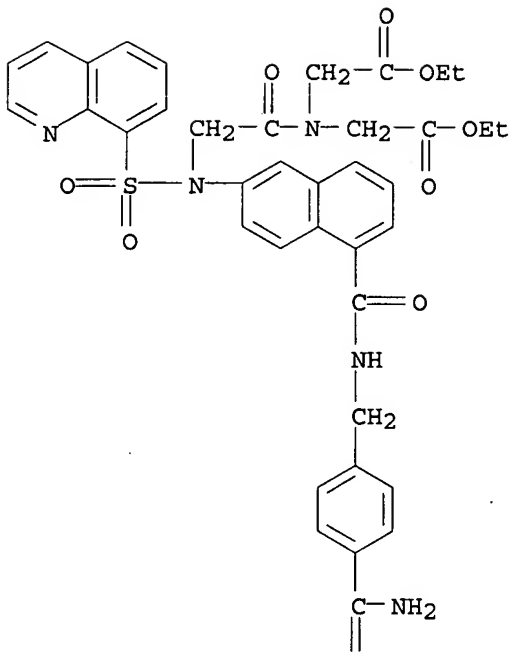


RN 227276-69-9 CAPLUS
CN Glycine, N-[5-[[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



RN 227276-71-3 CAPLUS
CN Glycine, N-[5-[[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-(2-ethoxy-2-oxoethyl)-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

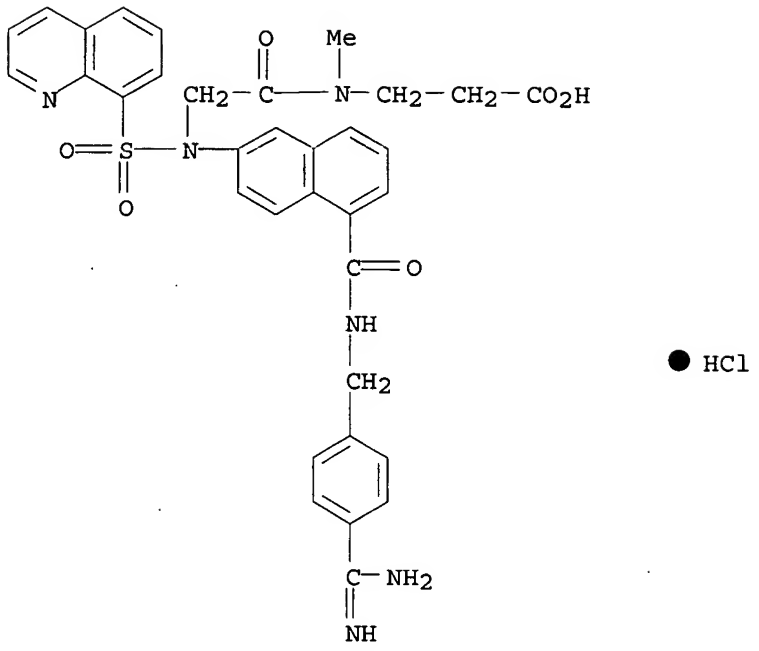
PAGE 1-A



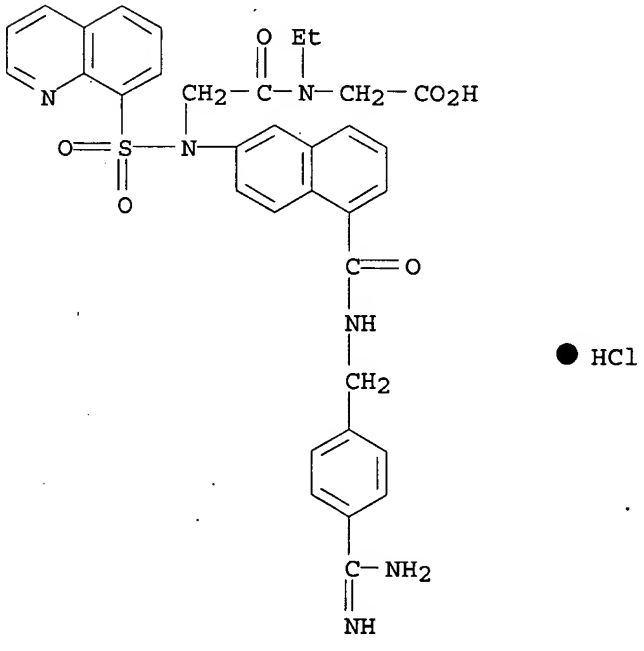
PAGE 2-A

● HCl

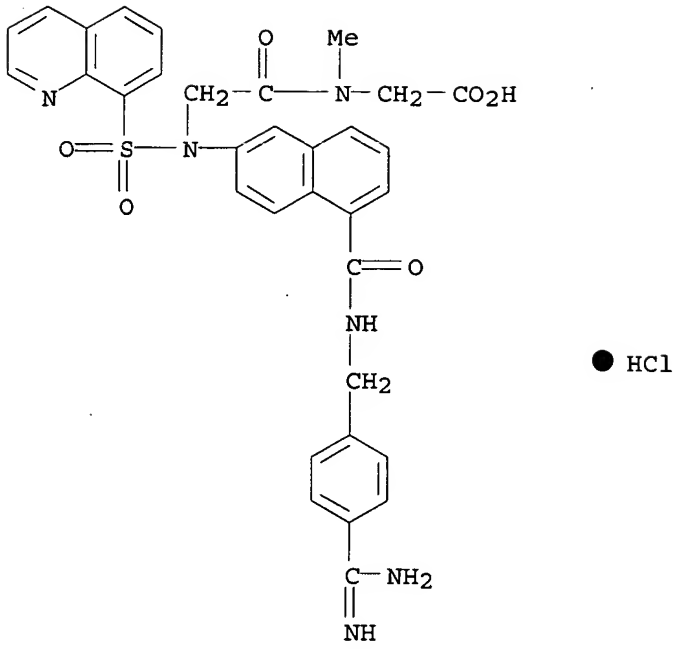
RN 227276-76-8 CAPLUS
CN β-Alanine, N-[5-[[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



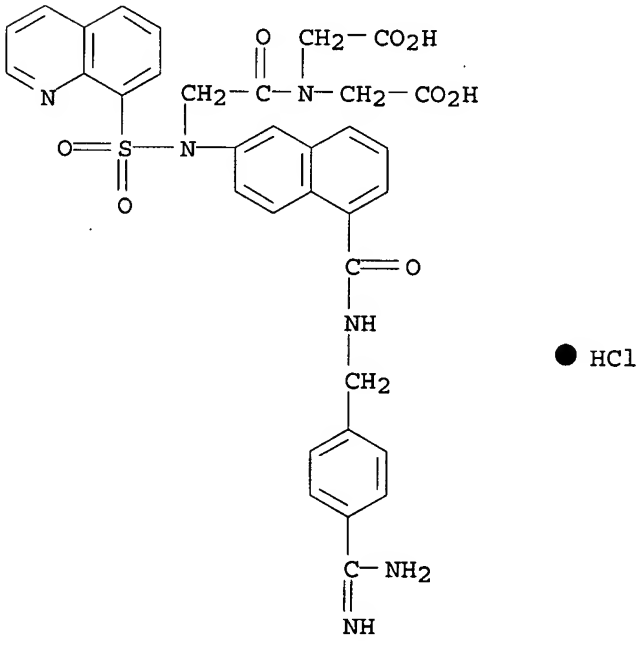
RN 227276-78-0 CAPLUS
CN Glycine, N-[5-[[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-ethyl-, monohydrochloride (9CI) (CA INDEX NAME)



RN 227276-79-1 CAPLUS
CN Glycine, N-[5-[[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

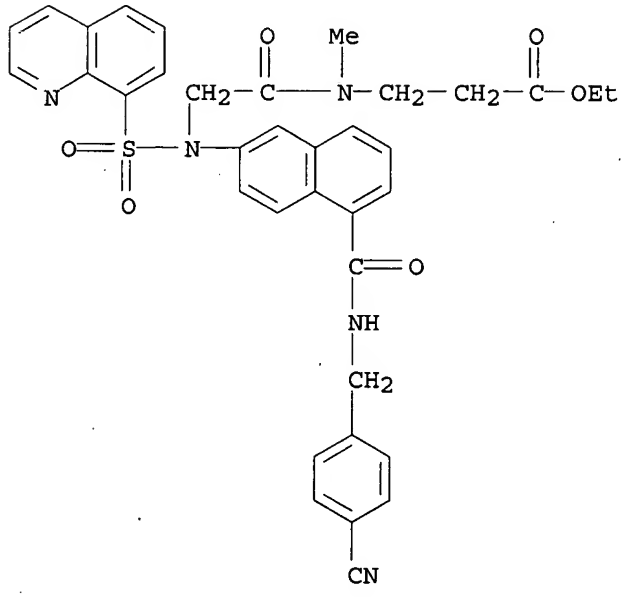


RN 227276-81-5 CAPLUS
CN Glycine, N-[5-[[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-(carboxymethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

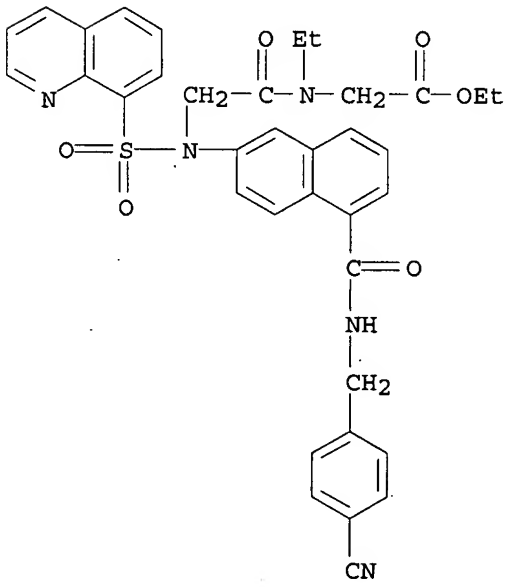


IT 227279-02-9 227279-04-1 227279-05-2
227279-07-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of carbamoylnaphthalenes as thrombin inhibitors)
RN 227279-02-9 CAPLUS
CN β-Alanine, N-[5-[[[(4-cyanophenyl)methyl]amino]carbonyl]-2-

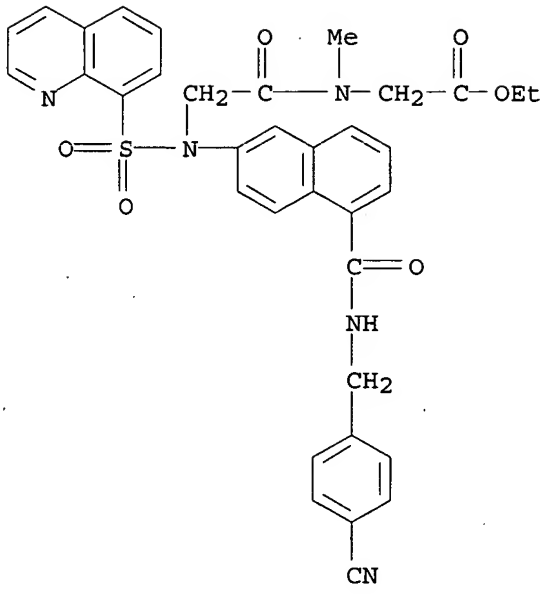
naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



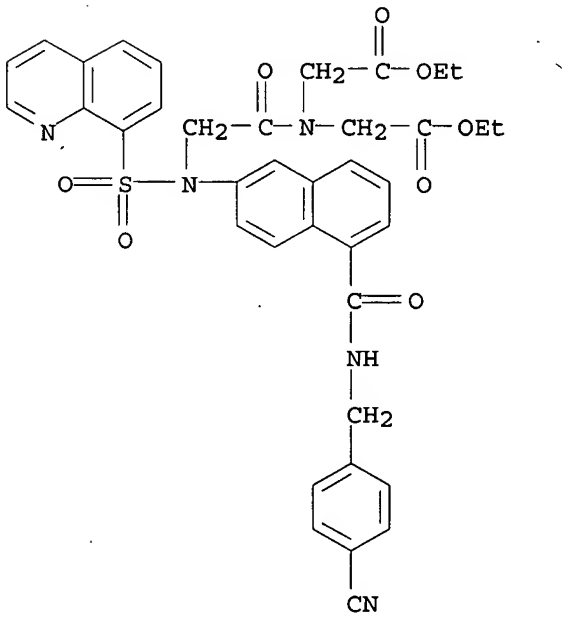
RN 227279-04-1 CAPLUS
CN Glycine, N-[5-[[[(4-cyanophenyl)methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-ethyl-, ethyl ester (9CI) (CA INDEX NAME)



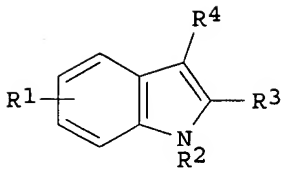
RN 227279-05-2 CAPLUS
CN Glycine, N-[5-[[[(4-cyanophenyl)methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 227279-07-4. CAPLUS
CN Glycine, N-[5-[[[(4-cyanophenyl)methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-(2-ethoxy-2-oxoethyl)-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
GI



I

AB Title compds. [I; R1 = F, Cl, Br, CO2H, aminocarbonyl, aminosulfonyl, amino, group convertible to CO2H in vivo; 1 of R2, R4 = (CO2H- or group convertible to CO2H in vivo-substituted) alkyl, the other = R5A; A = (CO2H- or group convertible to CO2H in vivo-substituted) alkylene, etc.; R5 = R6NHC(:NH)-substituted Ph; R4 = H, alkyl; R6 = H, in vivo-cleavable group], were prepared as antithrombotics with inhibitory activity against serine proteases XII and fibrinogen receptors. Thus, 3-[3-(4-amidinophenyl)propionyl]-1-methylindole-5-carboxylic acid N-(2-carboxyethyl)-N-phenylamide hydrochloride (preparation given) showed a thrombin time ED200 = 0.80 μM.

ACCESSION NUMBER: 1999:375527 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 131:31874
TITLE: Preparation of amidinophenylpropionylindoles and related compounds as thrombin inhibitors.
INVENTOR(S): Heckel, Armin; Walter, Rainer; Soyka, Rainer; Stassen, Jean-Marie; Wienen, Wolfgang; Binder, Klaus
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma KG, Germany
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9928297	A1	19990610	WO 1998-EP7661	19981127
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19753522	A1	19990610	DE 1997-19753522	19971203
AU 9922671	A	19990616	AU 1999-22671	19981127
PRIORITY APPLN. INFO.:			DE 1997-19753522 A	19971203
			WO 1998-EP7661 W	19981127

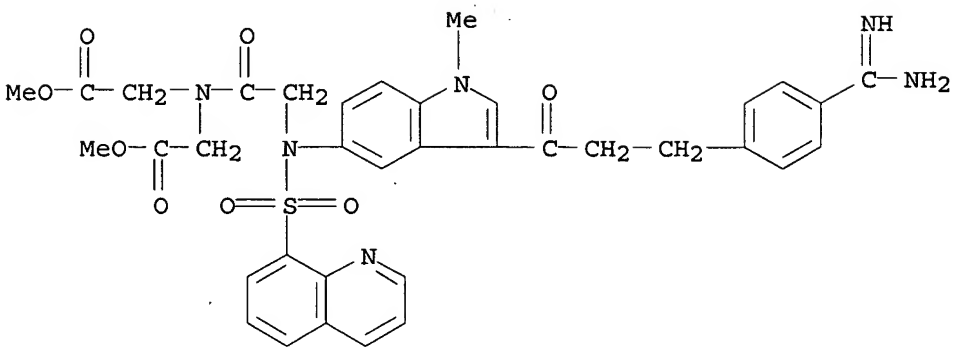
OTHER SOURCE(S): MARPAT 131:31874

IT 226899-02-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of amidinophenylpropionylindoles and related compds. as thrombin inhibitors)

RN 226899-02-1 CAPLUS
CN Glycine, N-[3-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-(2-methoxy-2-oxoethyl)-, methyl ester, monoacetate (9CI) (CA INDEX NAME)

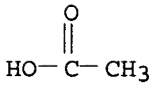
CM 1

CRN 226899-01-0
CMF C36 H36 N6 O8 S

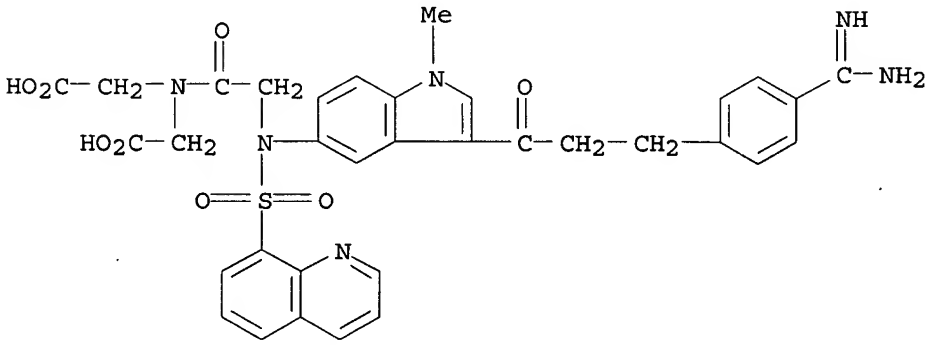


CM 2

CRN 64-19-7
CMF C2 H4 O2

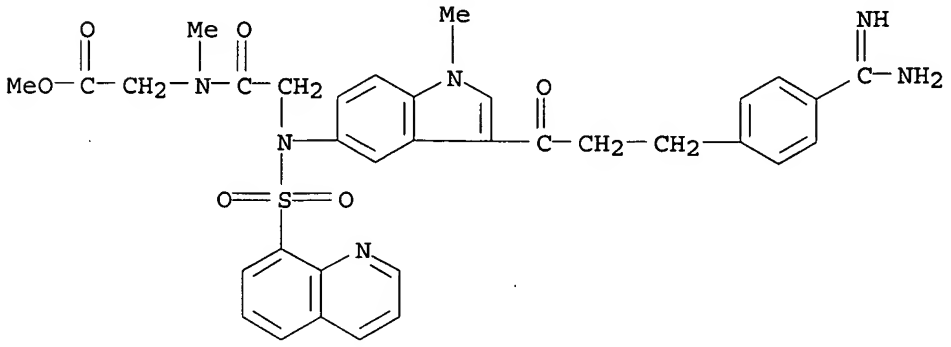


IT 226899-05-4P 226899-11-2P 226899-13-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amidinophenylpropionylindoles and related compds. as thrombin inhibitors)
RN 226899-05-4 CAPLUS
CN Glycine, N-[3-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-(carboxymethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



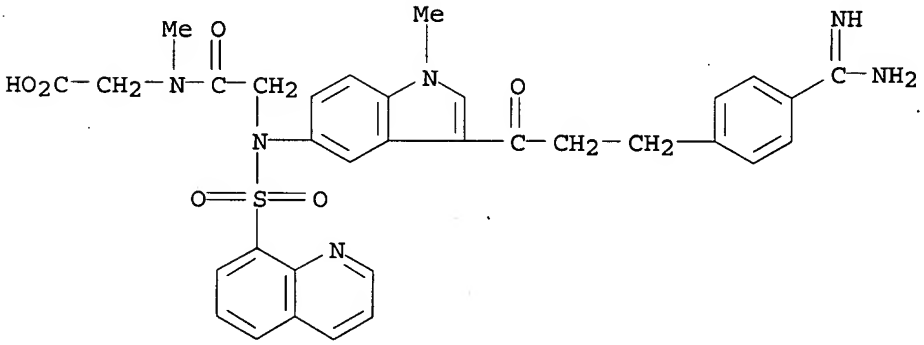
● HCl

RN 226899-11-2 CAPLUS
CN Glycine, N-[3-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, methyl ester, monohydriodide (9CI) (CA INDEX NAME)



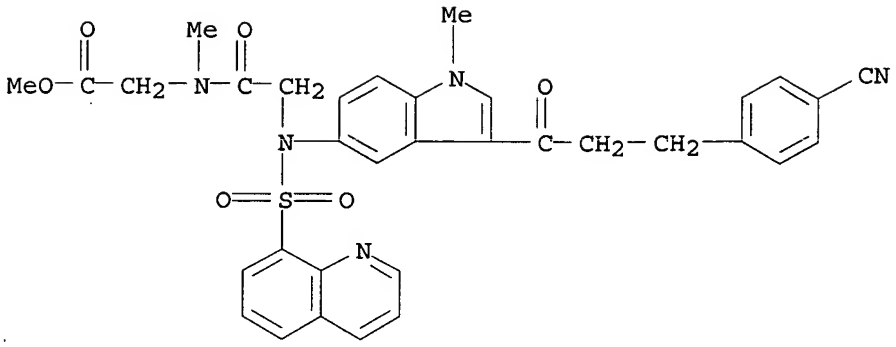
● HI

RN 226899-13-4 CAPLUS
CN Glycine, N-[3-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

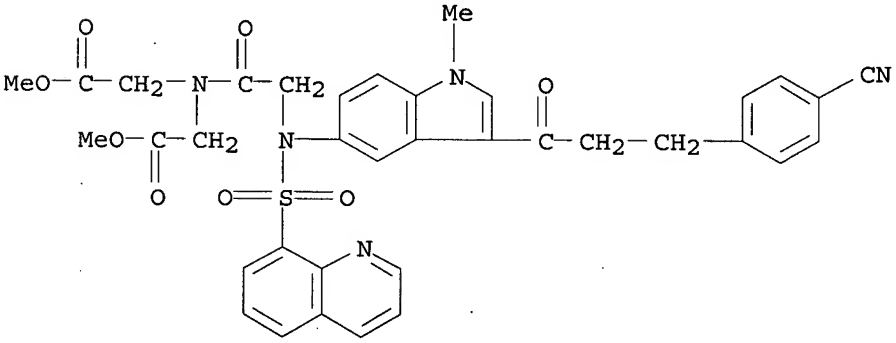


● HCl

IT 226902-20-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amidinophenylpropionylindoles and related compds. as thrombin inhibitors)
RN 226902-20-1 CAPLUS
CN Glycine, N-[3-[3-(4-cyanophenyl)-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

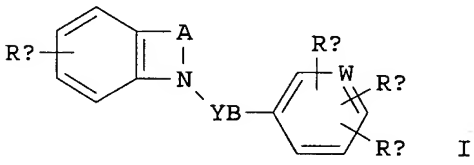


IT 226901-00-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amidinophenylpropionylindoles and related compds. as thrombin inhibitors)
RN 226901-00-4 CAPLUS
CN Glycine, N-[3-[3-(4-cyanophenyl)-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-(2-methoxy-2-oxoethyl)-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
GI



I

AB Title compds. [I; Ra = H, NO2, amino, aminocarbonyl; Rb = cyano, aminomethyl, (substituted) amidino; Rc, Rd = H, F, Cl, Br, iodo, Me, MeO, NO2, amino; A = (substituted) ethylene, ethyenylene, propylene, etc.; B = bond, (substituted) methylene, ethylene, ethenylene, propylene, etc.; W =

N, CH; Y = CH2, CO, CS], were prepared Thus, 1-[3-(4-amidinophenyl)propionyl]-1,2,3,4-tetrahydroquinoline-6-carboxylic acid methyl-N-phenylamide (preparation given) had a thrombin time ED200 = 0.02 μM.

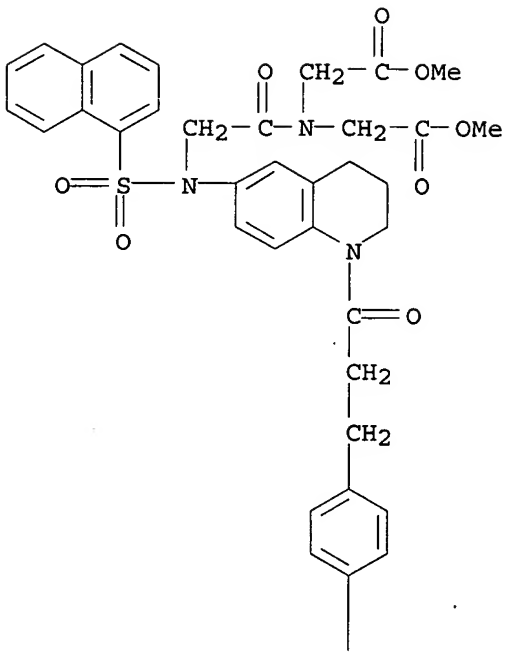
ACCESSION NUMBER: 1999:35065 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 130:110166
TITLE: Preparation of amidinophenylpropionyltetrahydroquinolines and related compounds as antithrombotics.
INVENTOR(S): Heckel, Armin; Soyka, Rainer; Grell, Wolfgang; Haaksma, Eric; Binder, Klaus; Zimmermann, Rainer
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany
SOURCE: Ger. Offen., 50 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19727117	A1	19990107	DE 1997-19727117	19970626
CA 2288744	A1	19990107	CA 1998-2288744	19980622
WO 9900371	A1	19990107	WO 1998-EP3800	19980622
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9887279	A	19990119	AU 1998-87279	19980622
EP 991624	A1	20000412	EP 1998-938621	19980622
EP 991624	B1	20031119		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002511088	T	20020409	JP 1999-505265	19980622
AT 254602	T	20031215	AT 1998-938621	19980622
MX 9911261	A	20000630	MX 1999-11261	19991206
US 6300342	B1	20011009	US 1999-457961	19991209

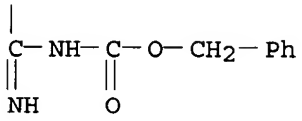
PRIORITY APPLN. INFO.: DE 1997-19727117 A 19970626
WO 1998-EP3800 W 19980622

OTHER SOURCE(S): MARPAT 130:110166
IT 219642-91-8P 219645-27-9P 219645-55-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amidinophenylpropionyltetrahydroquinolines and related compds. as antithrombotics)
RN 219642-91-8 CAPLUS
CN Glycine, N-(1-naphthalenylsulfonyl)-N-[1,2,3,4-tetrahydro-1-[3-[4-[imino[[(phenylmethoxy)carbonyl]amino]methyl]phenyl]-1-oxopropyl]-6-quinolinyl]glycyl-N-(2-methoxy-2-oxoethyl)-, methyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



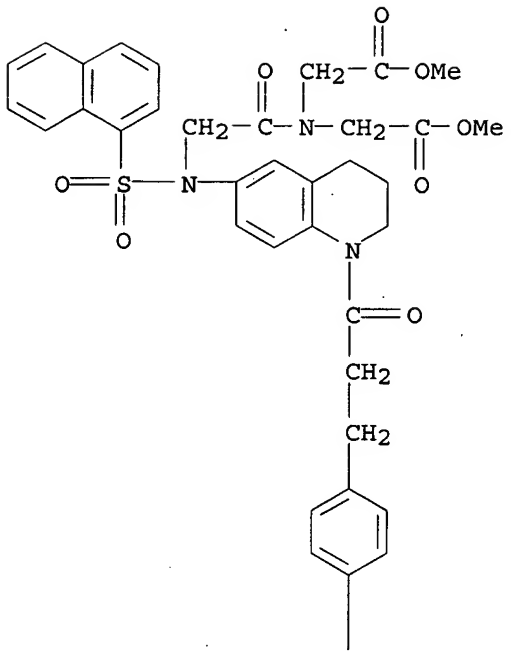
PAGE 2-A



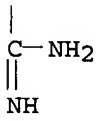
RN 219645-27-9 CAPLUS

CN Glycine, N-[1-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1,2,3,4-tetrahydro-6-quinolinyl]-N-(1-naphthalenylsulfonyl)glycyl-N-(2-methoxy-2-oxoethyl)-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



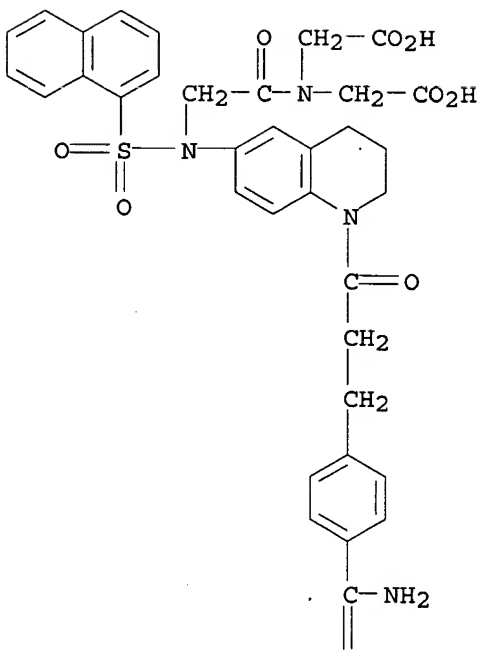
PAGE 2-A



● HCl

RN 219645-55-3 CAPLUS
CN Glycine, N-[1-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1,2,3,4-tetrahydro-6-quinolinyl]-N-(1-naphthalenylsulfonyl)glycyl-N-(carboxymethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



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● HCl

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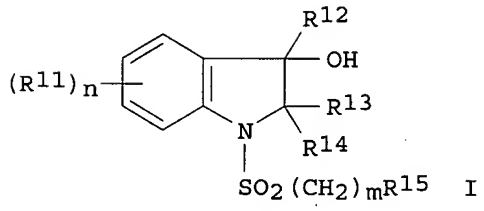


AB Title compds. I (R'1 = halo, C1-4 alkyl, HO, C1-4 alkoxy, PhCH2O, NC, F3C, O2N, H2N; R'2 = C1-6 alkyl, C3-7 cycloalkyl, C5-7 cycloalkylene, (substituted) Ph, etc.; R'3 = H; R'4 = H2NCO, R'6R'7NCO wherein R'6R'7N = saturated 5-membered substituted N-heterocyclyl; R'5 = C1-4 alkyl, 1-, 2-naphthyl, (substituted) Ph, etc.; n = m = 0-2) or a salt thereof, are prepared CH2BrCONMe2 (preparation given) and 5-chloro-2-(tosylamino)phenyl cyclohexyl ketone were reacted to give

2-[N-tosyl-N-(dimethylcarbamoylmethyl)amino]-5-(chlorophenyl) cyclohexyl ketone which in THF was treated with Li diisopropylamide to give after workup trans-I (R'1n = 5-Cl, R'2 = cyclohexyl, R'3 = H, R'4 = Me2NCO, R'5 = 4-MeC6H4, m = 0). The IC50 of I affinity for oxytocin receptors was 10-5-10-8M.

ACCESSION NUMBER: 1995:777639 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 123:198616
TITLE: Preparation of N-sulfonylindoline derivatives with affinity for vasopressin and oxytocin receptors
INVENTOR(S): Wagnon, Jean; de Cointet, Paul; Nisato, Dino; Plouzane, Claude; Sereadeil-Legal, Claudine; Tonnerre, Bernard
PATENT ASSIGNEE(S): Elf Sanofi SA, Fr.
SOURCE: U.S., 50 pp. Cont.-in-part of U.S. Ser. No.737,655, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5338755	A	19940816	US 1992-923839	19920803
FR 2665441	A1	19920207	FR 1990-9778	19900731
FR 2665441	B1	19921204		
IL 114934	A	19960804	IL 1991-114934	19910730
HU 219351	B	20010328	HU 1971-99045	19910731
FR 2679903	A1	19930205	FR 1991-9908	19910802
FR 2679903	B1	19931203		
AU 9224758	A	19930302	AU 1992-24758	19920731
AU 658664	B2	19950427		
BR 9205336	A	19931116	BR 1992-5336	19920731
JP 06501960	T	19940303	JP 1993-503337	19920731
RU 2104268	C1	19980210	RU 1993-5168	19920731
IL 117592	A	19990411	IL 1992-117592	19920731
CZ 288173	B6	20010516	CZ 1993-682	19920731
CA 2206776	C	20020226	CA 1992-2206776	19920731
SK 283463	B6	20030805	SK 1993-426	19920731
NO 9301262	A	19930526	NO 1993-1262	19930401
NO 180047	B	19961028		
NO 180047	C	19970205		
FI 104069	B	19991115	FI 1993-1476	19930401
FI 104069	B1	19991115		
US 5397801	A	19950314	US 1994-240360	19940510
US 5481005	A	19960102	US 1994-348150	19941128
US 5578633	A	19961126	US 1995-458614	19950602
FI 9800175	A	19980127	FI 1998-175	19980127
FI 107048	B1	20010531		

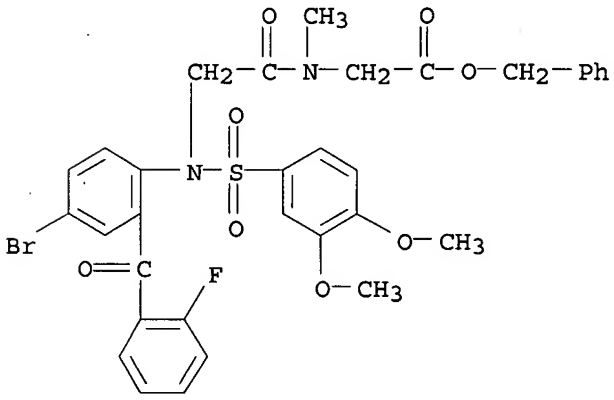
PRIORITY APPLN. INFO.:

FR 1990-9778	A	19900731
US 1991-737655	B2	19910730
FR 1991-9908	A	19910802
IL 1991-99012	A3	19910730
HU 1991-2552	A	19910731
CA 1992-2093221	A3	19920731
CS 1993-682	A	19920731
IL 1992-102703	A3	19920731
WO 1992-FR758	A	19920731
US 1992-923839	A3	19920803
FI 1993-1476	A	19930401
US 1993-923839	A3	19930803
US 1994-240360	A3	19940510
US 1994-348150	A3	19941128

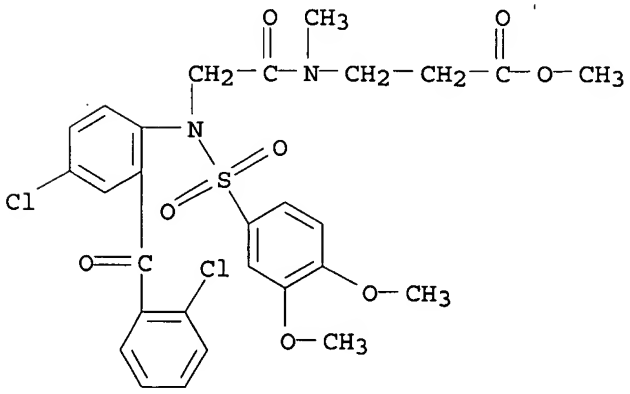
OTHER SOURCE(S): MARPAT 123:198616

IT 149152-33-0P 149152-34-1P 149152-35-2P
149152-36-3P 149152-39-6P 149152-40-9P
149152-42-1P 149152-43-2P 149152-44-3P
167400-68-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-sulfonylindoline derivs. with affinity for vasopressin and oxytocin receptors)

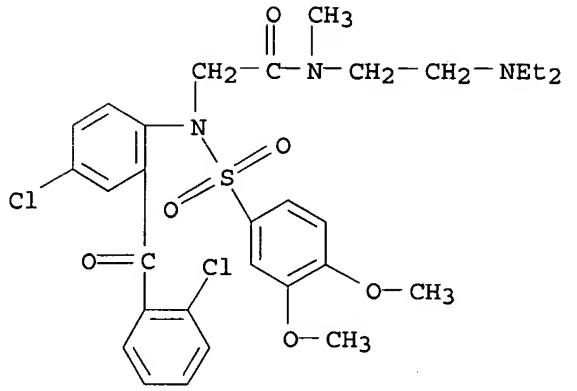
RN 149152-33-0 CAPLUS
CN Glycine, N-[N-[4-bromo-2-(2-fluorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



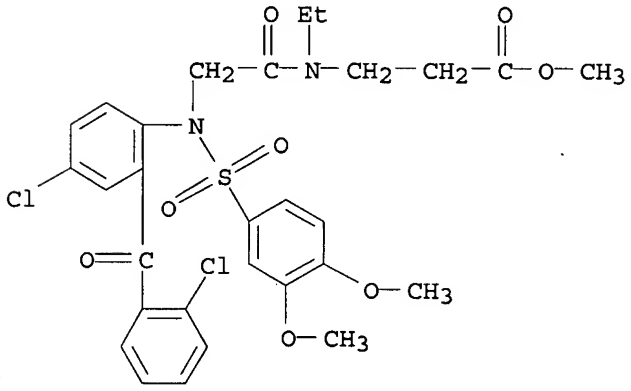
RN 149152-34-1 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



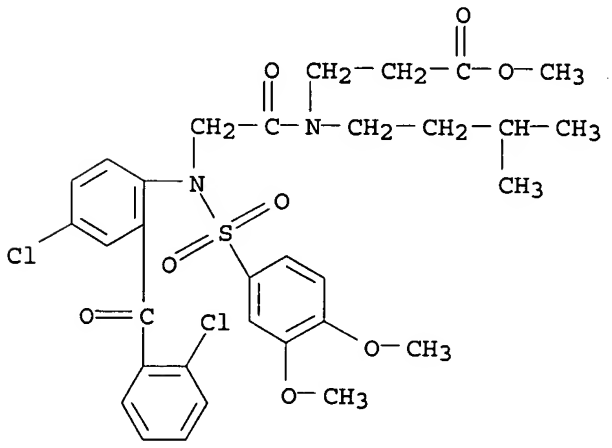
RN 149152-35-2 CAPLUS
CN Acetamide, 2-[[4-chloro-2-(2-chlorobenzoyl)phenyl][(3,4-dimethoxyphenyl)sulfonyl]amino]-N-[2-(diethylamino)ethyl]-N-methyl- (9CI) (CA INDEX NAME)



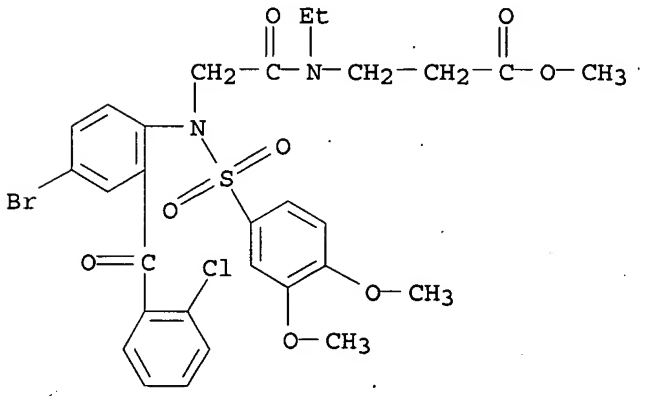
RN 149152-36-3 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



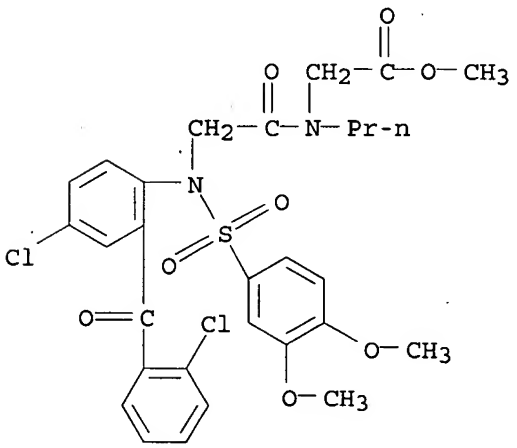
RN 149152-39-6 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(3-methylbutyl)-, methyl ester (9CI) (CA INDEX NAME)



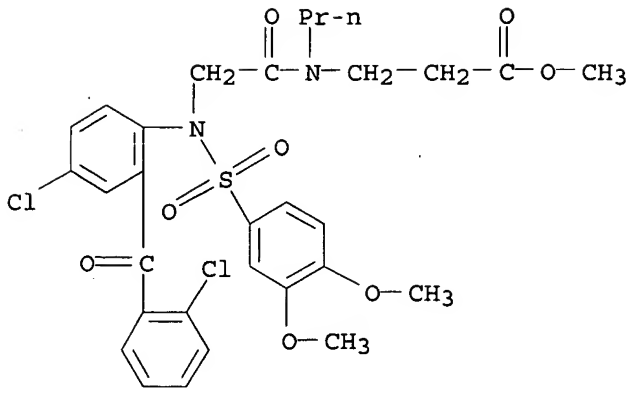
RN 149152-40-9 CAPLUS
CN β-Alanine, N-[N-[4-bromo-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



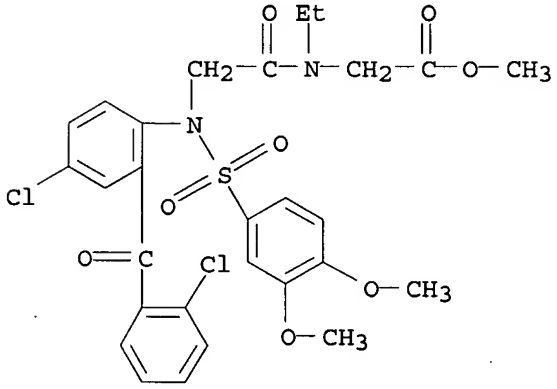
RN 149152-42-1 CAPLUS
CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-propyl-, methyl ester (9CI) (CA INDEX NAME)



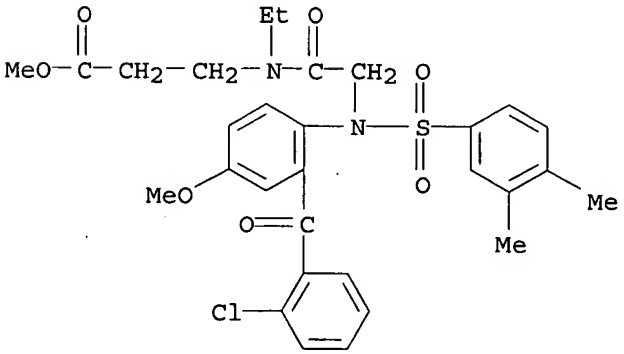
RN 149152-43-2 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-propyl-, methyl ester (9CI) (CA INDEX NAME)



RN 149152-44-3 CAPLUS
CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



RN 167400-68-2 CAPLUS
CN β-Alanine, N-[N-[2-(2-chlorobenzoyl)-4-methoxyphenyl]-N-[(3,4-dimethylphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



IT 149152-22-7P 149152-26-1P 149152-31-8P
149152-48-7P 149152-51-2P 167400-91-1P

167400-95-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-sulfonylindoline derivs. with affinity for vasopressin and oxytocin receptors)

RN 149152-22-7 CAPLUS
CN Acetamide, 2-[[4-chloro-2-(2-chlorobenzoyl)phenyl][(3,4-dimethoxyphenyl)sulfonyl]amino]-N-methyl-N-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

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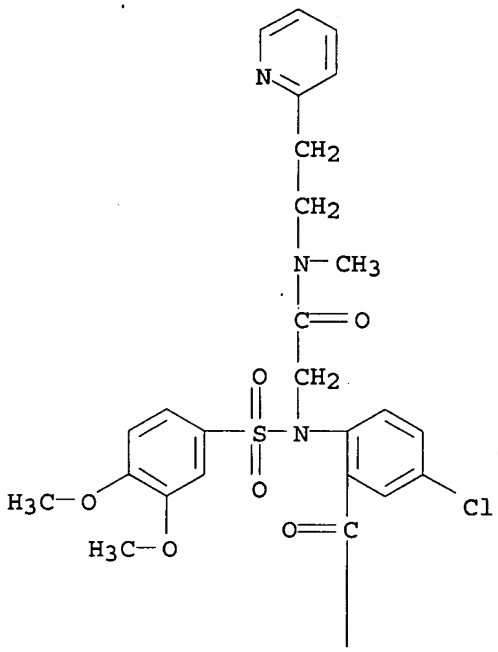

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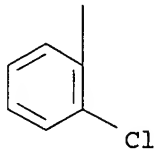
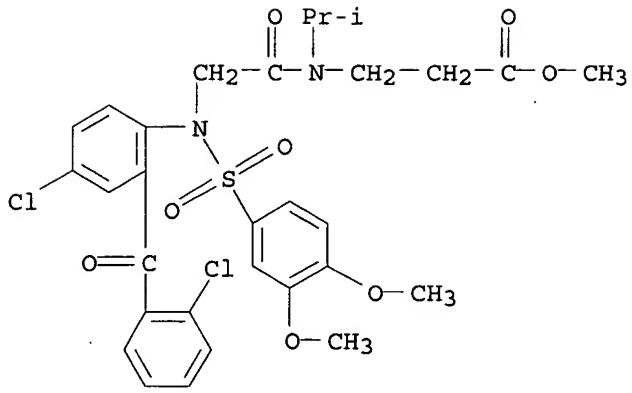
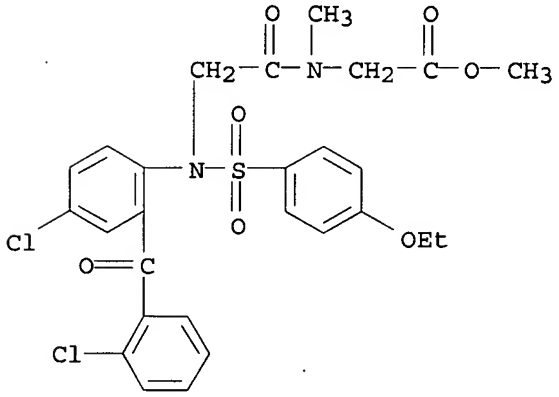


RN 149152-26-1 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)

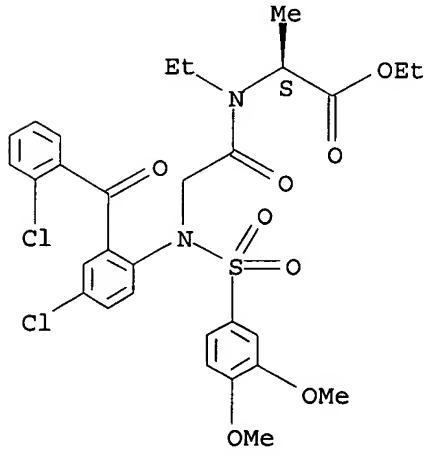


RN 149152-31-8 CAPLUS
CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(4-ethoxyphenyl)sulfonyl]glycyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

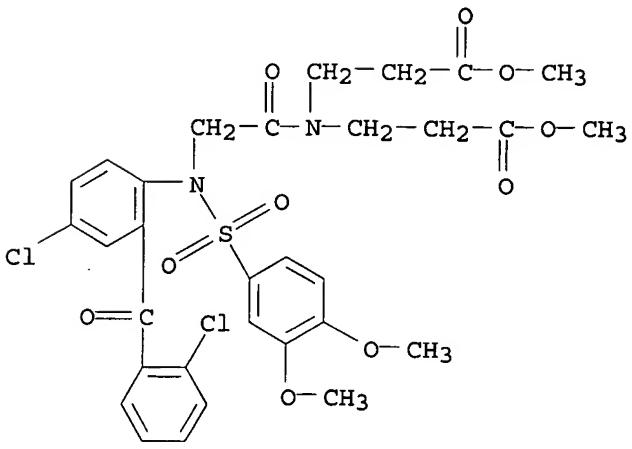


RN 149152-48-7 CAPLUS
CN L-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, ethyl ester (9CI) (CA INDEX NAME)

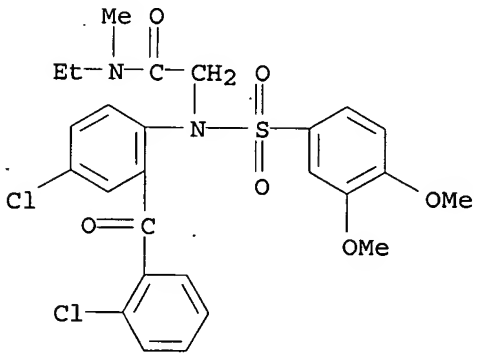
Absolute stereochemistry.



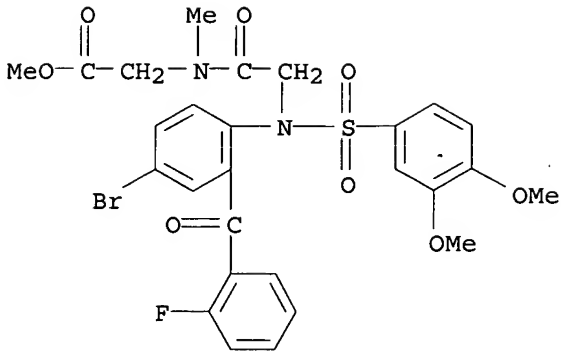
RN 149152-51-2 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(3-methoxy-3-oxopropyl)-, methyl ester (9CI) (CA INDEX NAME)



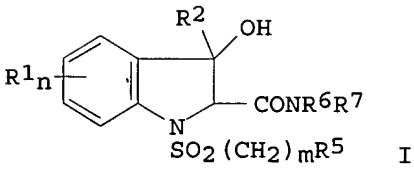
RN 167400-91-1 CAPLUS
CN Acetamide, 2-[[4-chloro-2-(2-chlorobenzoyl)phenyl][(3,4-dimethoxyphenyl)sulfonyl]amino]-N-ethyl-N-methyl- (9CI) (CA INDEX NAME)



RN 167400-95-5 CAPLUS
CN Glycine, N-[N-[4-bromo-2-(2-fluorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
GI



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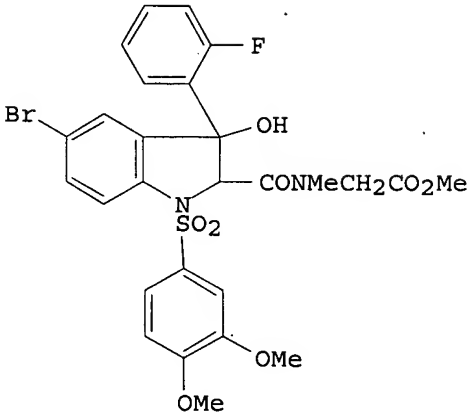


II

AB Title compds. [I; R1 = OH, halo, alkyl, alkoxy, etc.; R2 = (cyclo)alkyl, (nitro)phenyl, etc.; R5 = alkyl, (nitro)phenyl, naphthyl, etc.; R6 = alkyl; R6, R7 = 4-piperidinyl, 3-azetidinyl, etc.; NR6R7 = (thio)morpholino, thiazolidino, piperazino, etc.; m, n = 0-2] were prepared Thus, 2-amino-5-bromo-2'-fluorobenzophenone was amidated by 3,4-(MeO)2C6H3SO2Cl and the product N-alkylated by BrCH2CONMeCH2CO2Me to give, after cyclization of the product, title compound II. I had IC50 of 10-9, and 10-5 to 10-8 M, against vasopressin and oxytocin binding, resp., in vitro.

ACCESSION NUMBER: 1993:539091 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 119:139091
TITLE: Preparation of 1-phenylsulfonyl-3-hydroxyindoline-2-carboxamides as oxytocin and vasopressin antagonists
INVENTOR(S): Wagnon, Jean; Serradeil-Legal, Claudine; Tonnerre, Bernard; Plouzane, Claude; Nisato, Dino
PATENT ASSIGNEE(S): Elf Sanofi SA, Fr.
SOURCE: Eur. Pat. Appl., 71 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 526348	A1	19930203	EP 1992-402213	19920803
EP 526348	B1	19980218		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
FR 2679903	A1	19930205	FR 1991-9908	19910802
FR 2679903	B1	19931203		
CA 2093221	A1	19930203	CA 1992-2093221	19920731
CA 2093221	C	19980922		
WO 9303013	A1	19930218	WO 1992-FR758	19920731
W: AU, BR, CA, CS, FI, HU, JP, KR, NO, RU				
AU 9224758	A	19930302	AU 1992-24758	19920731
AU 658664	B2	19950427		
ZA 9205781	A	19930302	ZA 1992-5781	19920731
BR 9205336	A	19931116	BR 1992-5336	19920731
JP 06501960	T	19940303	JP 1993-503337	19920731
LT 3064	B	19941025	LT 1992-114	19920731
LV 10091	B	19950420	LV 1992-87	19920731
HU 68927	A2	19950828	HU 1993-951	19920731
IL 102703	A	19970318	IL 1992-102703	19920731
JP 2633085	B2	19970723	JP 1992-503337	19920731
RU 2104268	C1	19980210	RU 1993-5168	19920731
IL 117592	A	19990411	IL 1992-117592	19920731
CZ 288173	B6	20010516	CZ 1993-682	19920731
CA 2206776	C	20020226	CA 1992-2206776	19920731
SK 283463	B6	20030805	SK 1993-426	19920731
AT 163289	T	19980315	AT 1992-402213	19920803
ES 2117038	T3	19980801	ES 1992-402213	19920803
NO 9301262	A	19930526	NO 1993-1262	19930401
NO 180047	B	19961028		
NO 180047	C	19970205		
FI 104069	B	19991115	FI 1993-1476	19930401
FI 104069	B1	19991115		
US 5481005	A	19960102	US 1994-348150	19941128
AU 9511541	A	19950504	AU 1995-11541	19950203
AU 691223	B2	19980514		
HU 9500474	A3	19951030	HU 1995-474	19950628
FI 9800175	A	19980127	FI 1998-175	19980127
FI 107048	B1	20010531		

PRIORITY APPLN. INFO.:		
FR 1991-9908	A	19910802
FR 1990-9778	A	19900731
US 1991-737655	B2	19910730
CA 1992-2093221	A3	19920731
CS 1993-682	A	19920731
IL 1992-102703	A3	19920731
WO 1992-FR758	A	19920731
FI 1993-1476	A	19930401
US 1993-923839	A3	19930803
US 1994-240360	A3	19940510

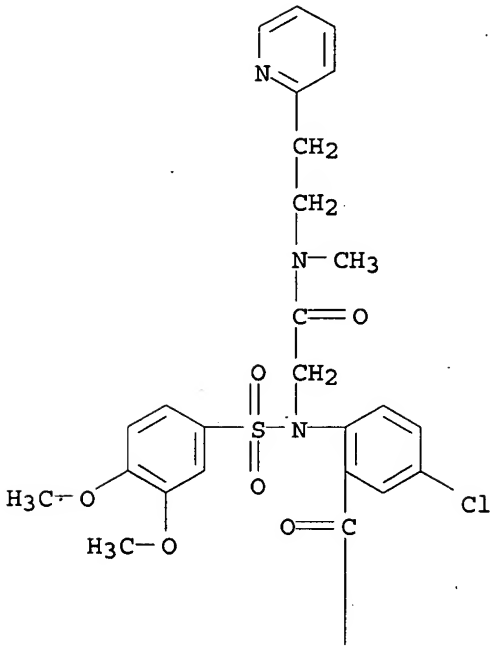
OTHER SOURCE(S): MARPAT 119:139091

IT 149152-22-7P 149152-26-1P 149152-31-8P
149152-33-0P 149152-34-1P 149152-35-2P
149152-36-3P 149152-38-5P 149152-39-6P
149152-40-9P 149152-42-1P 149152-43-2P
149152-44-3P 149152-48-7P 149152-51-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of oxytocin and vasopressin antagonists)

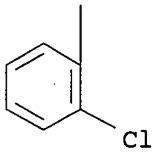
RN 149152-22-7 CAPLUS

CN Acetamide, 2-[[4-chloro-2-(2-chlorobenzoyl)phenyl][(3,4-dimethoxyphenyl)sulfonyl]amino]-N-methyl-N-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

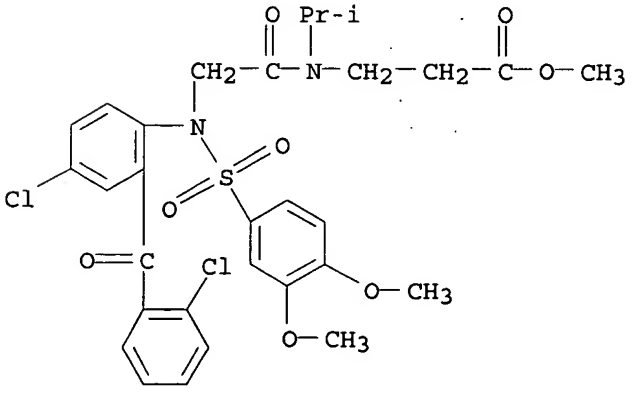
PAGE 1-A



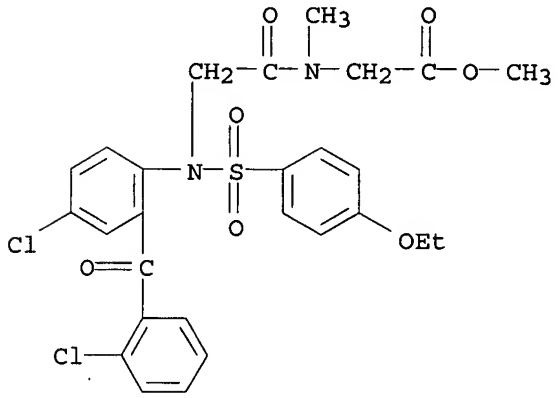
PAGE 2-A



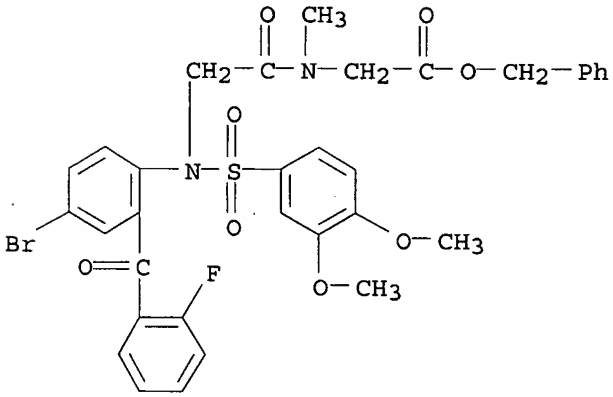
RN 149152-26-1 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(1-methylethyl)-, methyl ester (9CI) (CA INDEX NAME)



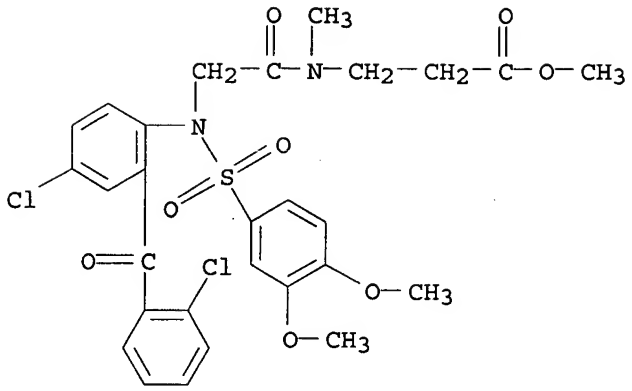
RN 149152-31-8 CAPLUS
CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(4-ethoxyphenyl)sulfonyl]glycyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



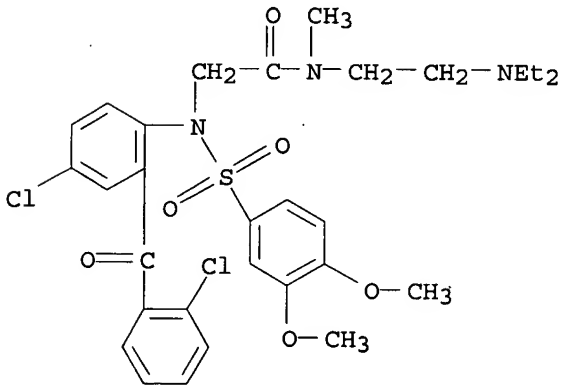
RN 149152-33-0 CAPLUS
CN Glycine, N-[N-[4-bromo-2-(2-fluorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



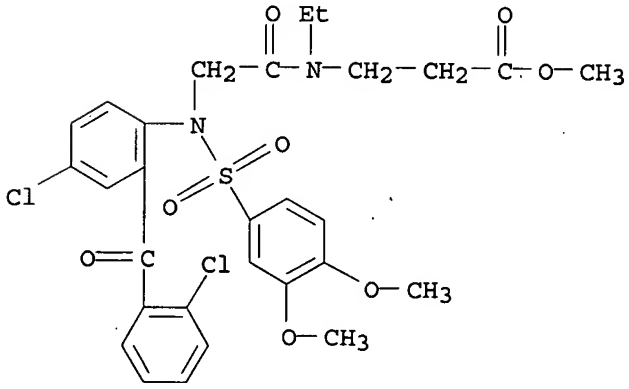
RN 149152-34-1 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 149152-35-2 CAPLUS
CN Acetamide, 2-[[4-chloro-2-(2-chlorobenzoyl)phenyl][(3,4-dimethoxyphenyl)sulfonyl]amino]-N-[2-(diethylamino)ethyl]-N-methyl- (9CI) (CA INDEX NAME)

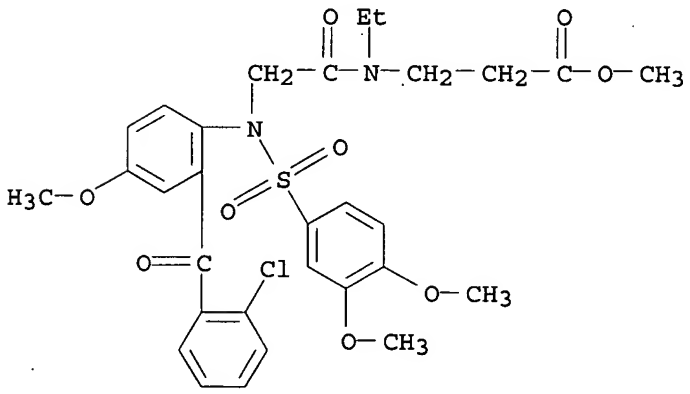


RN 149152-36-3 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)

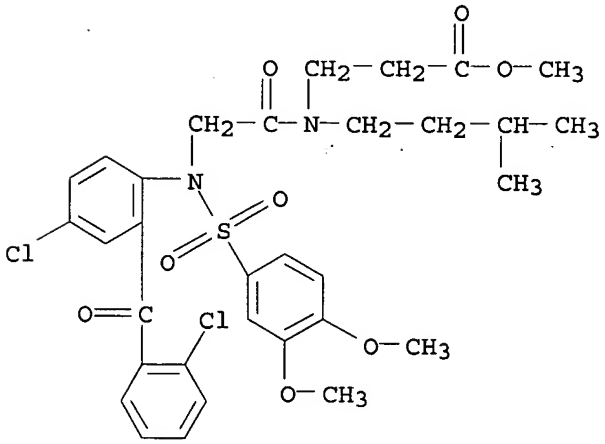


RN 149152-38-5 CAPLUS

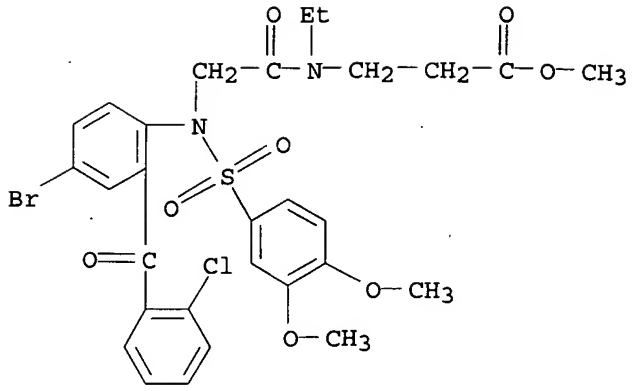
CN β-Alanine, N-[N-[2-(2-chlorobenzoyl)-4-methoxyphenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



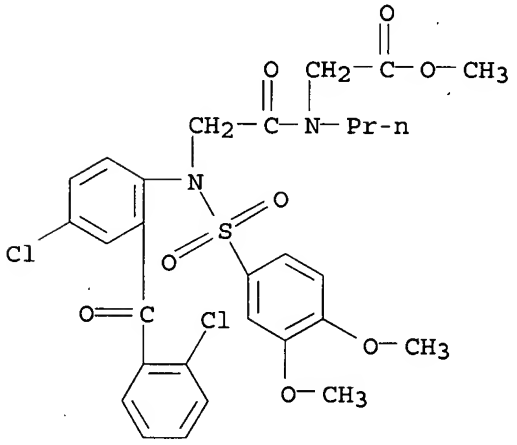
RN 149152-39-6 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(3-methylbutyl)-, methyl ester (9CI) (CA INDEX NAME)



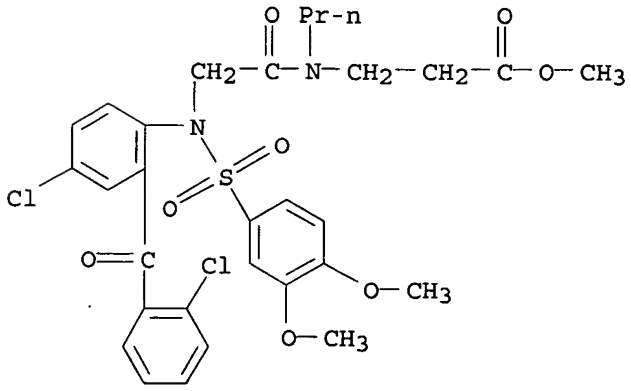
RN 149152-40-9 CAPLUS
CN β-Alanine, N-[N-[4-bromo-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



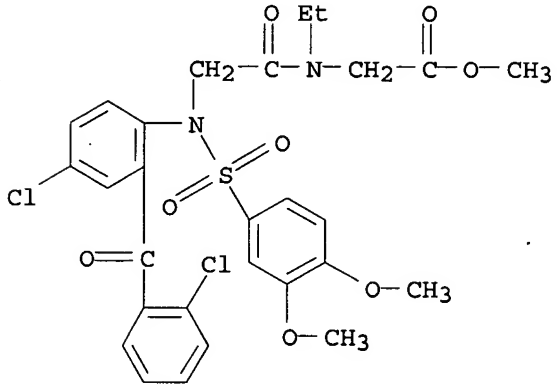
RN 149152-42-1 CAPLUS
CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-propyl-, methyl ester (9CI) (CA INDEX NAME)



RN 149152-43-2 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-propyl-, methyl ester (9CI) (CA INDEX NAME)

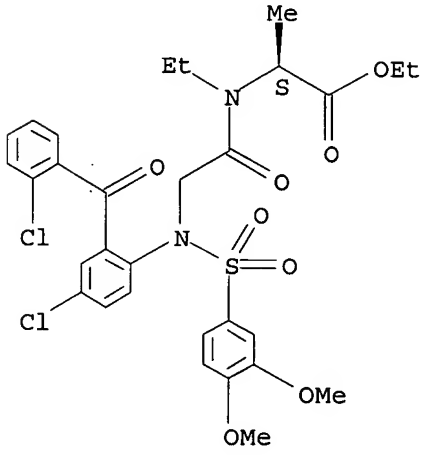


RN 149152-44-3 CAPLUS
CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)

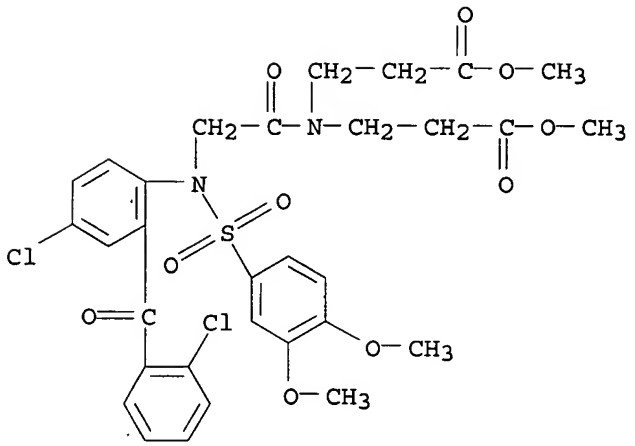


RN 149152-48-7 CAPLUS
CN L-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 149152-51-2 CAPLUS
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(3-methoxy-3-oxopropyl)-, methyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

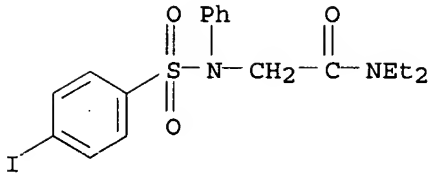
AB RSO2NHR' in aqueous NaOH (50% excess), treated with an equimolar amount of R''2NCSCl at 5° and the mixture stirred 2 hrs. at 20° gave the following RSO2NR'CSNR"2 (% yield, R, R', R", and m.p. shown): 54.2, Me, Ph, Me, 119-20°; 85.3, Et, Ph, Me, 101-2°; 87.1, Et, p-NCSC6H4, Et, 103-4°; 91.5, Ph, Ph, Me, 152-3°; 65.5, p-MeC6H4, p-ClC6H4, Me, 136-6.5°; 85.5, o-MeC6H4, Ph, Me, 124.5-5°; 86.3, iso-Pr, Ph, Et, 113-14°; 64.5, p-MeC6H4, Cl, Me, 149-50°; 91.6, p-FC6H4, Ph, Me, 151-2°; 62.7, p-ClC6H4, Ph, Me, 161-2°; 78.5, p-BrC6H4, Ph, Me, 154-5°; 52.7, p-IC6H4, Ph, Me, 156-7°. The p-iodophenyl member was prepared in Me2CO. Heating p-MeC6H4SO2NPhCSNMe2 with 40% H2SO4, 46 hrs. at 150° gave CSO, PhNH2, and Me2NH, as well as p-MeC6H4SO3H.

ACCESSION NUMBER: 1963:33089 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 58:33089
ORIGINAL REFERENCE NO.: 58:5567d-e
TITLE: Sulfanilides. II. N-Sulfonyl derivatives of urea
AUTHOR(S): Malinovskii, M. S.; Solomko, Z. F.; Glushko, L. P.
CORPORATE SOURCE: State Univ., Dnepropetrovsk
SOURCE: Zhurnal Obshchei Khimii (1962), 32, 728-31
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

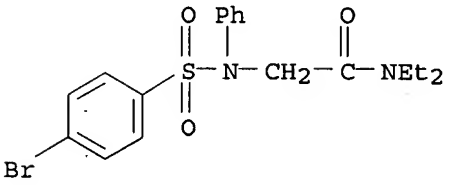
IT 88784-29-6P, Acetamide, N,N-diethyl-2-(p-iodo-N-phenylbenzenesulfonamido)- 93904-37-1P, Acetamide, 2-(p-bromo-N-phenylbenzenesulfonamido)-N,N-diethyl- 93995-09-6P, Acetamide, 2-(p-chloro-N-phenylbenzenesulfonamido)-N,N-diethyl- 93996-27-1P, Acetamide, N,N-diethyl-2-(p-nitro-N-phenylbenzenesulfonamido)- 94437-71-5P, Acetamide, N,N-diethyl-2-(N-phenyl-p-toluenesulfonamido)- 95167-60-5P, Acetamide, N,N-diethyl-2-(m-nitro-N-phenylbenzenesulfonamido)- 98981-10-3P, Acetamide, 2-(p-chloro-N-m-tolylbenzenesulfonamido)-N,N-diethyl-
RL: PREP (Preparation)
(preparation of)

RN 88784-29-6 CAPLUS

CN Acetamide, N,N-diethyl-2-(p-iodo-N-phenylbenzenesulfonamido)- (7CI) (CA INDEX NAME)



RN 93904-37-1 CAPLUS
CN Acetamide, 2-(p-bromo-N-phenylbenzenesulfonamido)-N,N-diethyl- (7CI) (CA INDEX NAME)



RN 93995-09-6 CAPLUS
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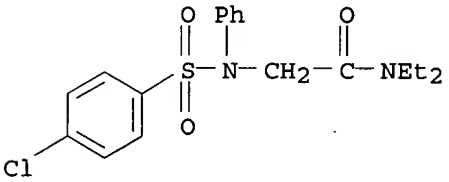

RN 93996-27-1 CAPLUS
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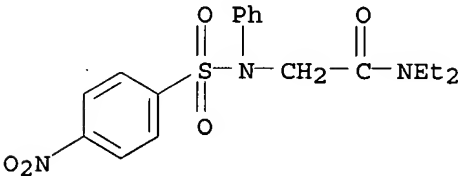
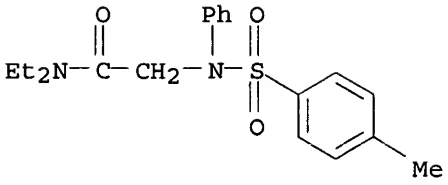
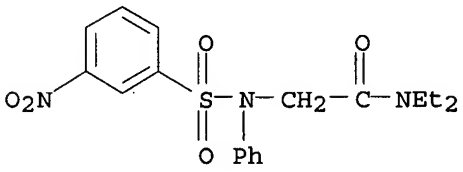


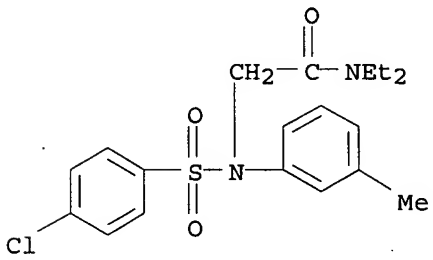
RN 94437-71-5 CAPLUS
CN Acetamide, N,N-diethyl-2-(N-phenyl-p-toluenesulfonamido)- (7CI) (CA INDEX NAME)



RN 95167-60-5 CAPLUS
CN Acetamide, N,N-diethyl-2-(m-nitro-N-phenylbenzenesulfonamido)- (7CI) (CA INDEX NAME)



RN 98981-10-3 CAPLUS
CN Acetamide, 2-(p-chloro-N-m-tolylbenzenesulfonamido)-N,N-diethyl- (7CI) (CA INDEX NAME)



L6 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
AB Addition of RSO2NHAr to aqueous NaOH (equimolar amount), followed by ClCH2CONEt2
in EtOH and 2-4 hrs. refluxing gave the following RSO2NArCH2CONEt2 (R, Ar, % yield and m.p. shown): Me, Ph, 60.6, 97-8°; Et, Ph, 57, 80-1°; Ph, Ph (I), 91.5, 93-4°; p-ClC6H4, Ph, 58, 117-18°; p-BrC6H4, Ph, 65.2, 102.5-3°; p-IC6H4, Ph, 44.5, 150.5-1°; p-ClC6H4, m-MeC6H4, 80.5, 77-8°; p-O2NC6H4, Ph, 46.5, 148-8.5° m-O2NC6H4, Ph, 72.3, 134-4.5°; p-MeC6H4, Ph, 95, 128-9% Heating PhNH2 with ClCH2CONEt2 in BuOH in the presence of Na2CO3 8-10 hrs. gave 39.2% PhNHCH2CONEt2, b4 175-82° (U.S. 2,568,142, CA 46, 3568a), which, heated with NaOAc in 30% EtOH to 70°, and treated with PhSO2Cl over 1 hr. gave I.

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TITLE: Sulfanilides. I. N-Sulfonylarylglycine dialkylamides
AUTHOR(S): Malinovskii, M. S.; Solomko, Z. F.; Teslenko, E. P.; Efremova, A. L.
CORPORATE SOURCE: State Univ., Dnepropetrovsk
SOURCE: Zhurnal Obshchei Khimii (1962), 32, 726-8
CODEN: ZOKHA4; ISSN: 0044-460X

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IT 88784-29-6P, Acetamide, N,N-diethyl-2-(p-iodo-N-phenylbenzenesulfonamido)- 93904-37-1P, Acetamide, 2-(p-bromo-N-phenylbenzenesulfonamido)-N,N-diethyl- 93995-09-6P, Acetamide, 2-(p-chloro-N-phenylbenzenesulfonamido)-N,N-diethyl- 93996-27-1P, Acetamide, N,N-diethyl-2-(p-nitro-N-phenylbenzenesulfonamido)- 94263-24-8P, Acetamide, N,N-diethyl-2-(N-phenylbenzenesulfonamido)- 94437-71-5P, Acetamide, N,N-diethyl-2-(N-phenyl-p-toluenesulfonamido)- 95167-60-5P, Acetamide, N,N-diethyl-2-(m-nitro-N-phenylbenzenesulfonamido)- 98981-10-3P, Acetamide, 2-(p-chloro-N-m-tolylbenzenesulfonamido)-N,N-diethyl-
RL: PREP (Preparation)
(preparation of)

RN 88784-29-6 CAPLUS
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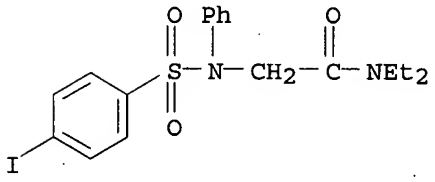

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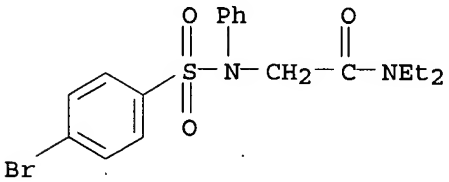

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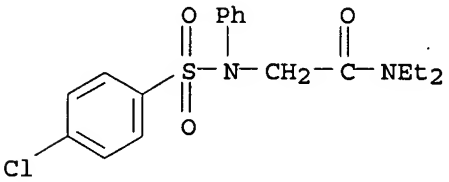

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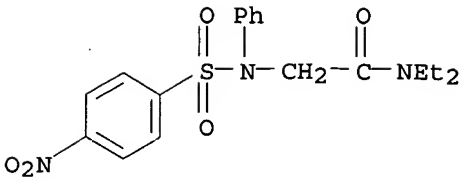

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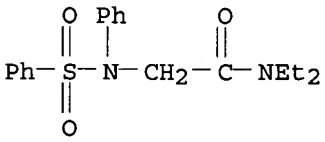

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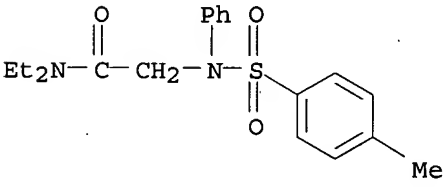

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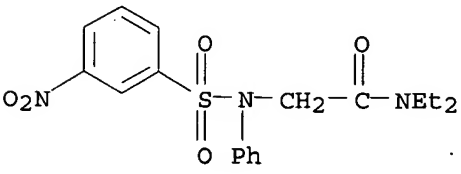

RN 98981-10-3 CAPLUS
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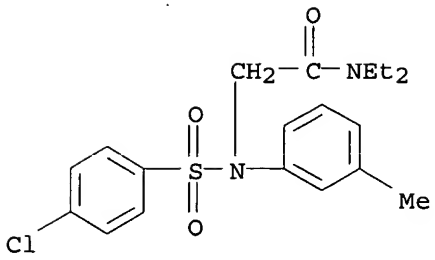
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CH2 — C — NEt2
O
S — N
O
Me
Cl